Integrated Greenhouse Gas Monitoring System for Germany (ITMS)

Overall Concept

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Christoph Gerbig[1], Andrea K. Kaiser-Weiss[2], Heinrich Bovensmann[3], Klaus Butterbach-Bahl[4], Christian Plass-Dülmer[2], Andreas Fix [5]

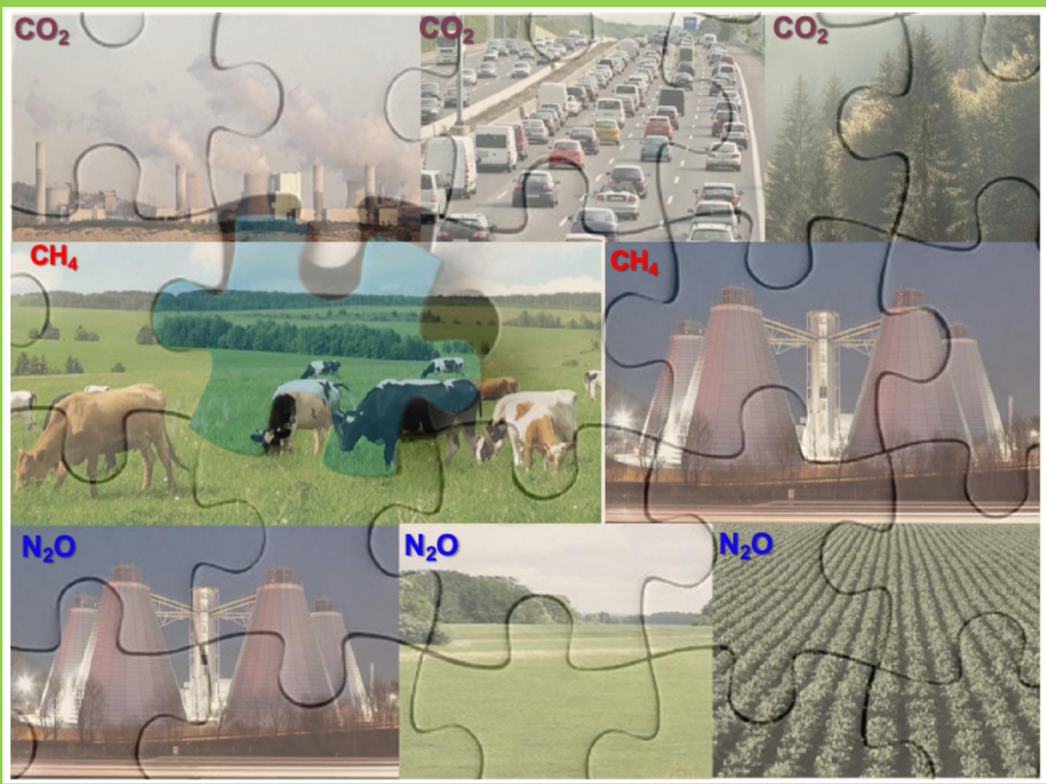
[1] Max-Planck-Institut für Biogeochemie, Jena

[2] Deutscher Wetterdienst, Offenbach am Main

[3] Institut für Umweltphysik, Universität Bremen

[4] Institut für Meteorologie und Klimaforschung, Atmosphärische Umweltforschung (IMK-IFU) des Karlsruher Instituts für Technologie (KIT)

[5] Institut für Physik der Atmosphäre, Deutsches Zentrum für Luft- und Raumfahrt



Based on the Community Document:

Integrated Greenhouse Gas Monitoring System for Germany (Work plan)

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by:

Main authors:

Christoph Gerbig[1], Andrea K. Kaiser-Weiss[2], Heinrich Bovensmann[3], Klaus Butterbach-Bahl[4], Christian Plass-Dülmer[2]

and contributing authors from the science community:

Almut Arneth[4], Sabrina Arnold[2], Christian Bernhofer[6], Heye Bogena[7], Nicolas Brüggemann[7], Christian Brümmer[8], Michael Buchwitz[3], John P. Burrows[3], Andre Butz [11], Jia Chen[20], Matthias Drösler[9], Gerhard Ehret[5], Alexander Graf[7], Thomas Grünwald[6], Dirk Günther[10], Samuel Hammer[11], Frank Hase[19], Martin Heimann[1], Mathias Herbst[2], Mario Hoppema[12], Frank Kaspar[2], Ralf Kiese[4], Alexander Knohl[13], Thomas Koch[2], Arne Körtzinger[14], Dagmar Kubistin[2], Ingeborg Levin[11], Matthias Lindauer[2], Buhalqem Mamtimin[2], Uta Moderow[6], Justus Notholt[3], Markus Rapp[5], Corinna Rebmann[15], Gregor Rehder[16], Markus Reichstein[1], Torsten Sachs[17], Klaus-Jürgen Schreiber[2], Lukas Siebicke[13], Tobias Steinhoff[14], Michael Strogies[10], Bernhard Vogel[18], Thorsten Warneke[3], Marion Wichmann-Fiebig[10]

[1] Max-Planck-Institut für Biogeochemie, Jena

[2] Deutscher Wetterdienst, Offenbach am Main

[3] Institut für Umweltphysik, Universität Bremen

[4] Institut für Meteorologie und Klimaforschung, Atmosphärische Umweltforschung (IMK-IFU) des Karlsruher Instituts für Technologie (KIT)

[5] Institut für Physik der Atmosphäre, Deutsches Zentrum für Luft- und Raumfahrt

[6] Institut für Hydrologie und Meteorologie, Technische Universität Dresden

[7] Institut für Bio- und Geowissenschaften Agrosphäre (IBG-3) des Forschungszentrum Jülich

[8] Thünen-Institut für Agrarklimaschutz und ICOS-D Konsortium

[9] Fachgebiet für Vegetationsökologie, Hochschule Weihenstephan-Triesdorf

[10] Umweltbundesamt, Standort Dessau

[11] Institut für Umweltphysik, Universität Heidelberg

[12] Alfred-Wegener-Institut Helmholtz Zentrum für für Polar- und Meeresforschung

[13] Abt. Bioklimatologie, Universität Göttingen

[14] GEOMAR, Helmholtz Zentrum für Ozeanforschung Kiel

[15] Helmholtz-Zentrum für Umweltforschung GmbH

[16] Leibniz Institut für Ostseeforschung Warnemünde

[17] Helmholtz-Zentrum Potsdam-Deutsches GeoForschungsZentrum

[18] Institut für Meteorologie und Klimaforschung, Department Troposphärenforschung (IMK-TRO) des KIT

[19] Institut für Meteorologie und Klimaforschung - Atmosphärische Spurengase und Fernerkundung (IMK-ASF) des KIT

[20] Fakultät für Elektrotechnik und Informationstechnik, Technische Universität München

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1. Introduction

The Integrated Greenhouse Gas Monitoring System – or in German: Integriertes Treibhausgas-Monitoringsystem (ITMS) – will enable Germany to operationally monitor the sources and sinks of the three most important long-lived greenhouse gases CO2, CH4, N2O with the help of independent measurements.

With the Paris Agreement (2015), the monitoring of greenhouse gases for climate protection was put into force at the political level. The Intergovernmental Panel on Climate Change (IPCC) and the United Nations Framework Convention on Climate Change (UNFCCC) recommend to supplement the national inventory reports with an observation-based monitoring of greenhouse gas emissions. The WMO Framework Integrated Global Greenhouse Gas Information System (IG3IS) develops recommendations for national contributions. The Integrated Greenhouse Gas Monitoring System (ITMS) implements the German contribution to the IG3IS.

The ITMS will establish on-line provision and visualization of the natural and anthropogenic sources and sinks of Germany's most important greenhouse gases (CO_2, CH_4, N_2O). It will provide adequate spatially and temporally resolved, sector-specific information. This supports the national reporting of the Federal Environment Agency UBA, as well as the scientific basis of certificate trading. Overestimations and underestimations of sources and sinks as well as regional hotspots can be detected and thus uncertainties can be reduced. Differentiation of natural and anthropogenic contributions, and quantification of diffuse sources and reductions of greenhouse gases, as in agriculture, forestry and other land uses (so-called AFOLU sector), but also in transport, will become possible. The ITMS also enables the evaluation and further development of observation strategies as well as support for other countries in this topic.

With the establishment of the operational ITMS service, the scientific measurement and modelling communities of Germany will be integrated, utilizing the Copernicus Services, the EU research projects, ICOS, IAGOS, as well as satellite data in a continuous manner. The long-term implementation of the ITMS research results at the operational authorities DWD, UBA and Thünen-Institute make the project efficient and sustainable.

In the long term, ITMS provides means for industry and policy consultation, tailored with regard to mitigation success.

2. Goals and Stakeholders

2.1 Ambition of ITMS

Developing an ITMS requires the operational implementation of data flows, data assimilation and inversion systems, and building on best possible model representations of all relevant processes involved in the greenhouse gas budgets. In addition to the research and development in these fields, the ITMS focus is to reduce and characterize uncertainties/errors introduced in the full processing chain, including development of observational data, models and a-priori databases.

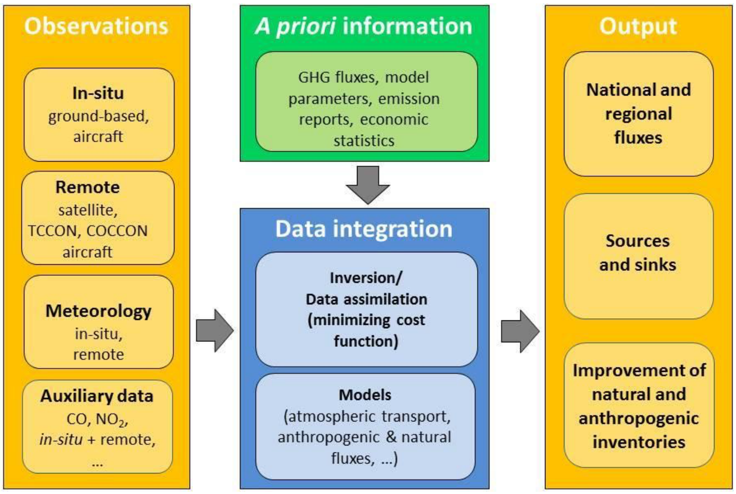

Figure 1: Components of the ITMS for Germany based on the European CO_2 Report [1]: observations (delivered by the observing systems community) and prior information (delivered by the flux community) are used with inversion models to estimate GHG sources and sinks.

Central critical elements of the ITMS are:

1) observational data streams from traceable and quality-controlled measurements of atmospheric GHG concentrations and surface-atmosphere fluxes,

2) first guess (a-priori) estimates of spatially and temporally resolved GHG fluxes from anthropogenic activities and natural processes, and

3) a data assimilation system that combines the information with atmospheric tracer transport modelling in a quantitative way to estimate GHG sources and sinks.

Data streams from in-situ observations are currently available from the Integrated Carbon Observation System (ICOS), from IAGOS (the In-service Aircraft for a Global Observing System), but data streams from satellites and ground based remote sensing need implementation and satellite data require special tailoring for the high resolution and regionally referenced application planned in ITMS. Prior information used in the data assimilation needs to be specific for Germany, compatible with the national GHG reporting, and involve bottom-up models that quantitatively use cutting edge activity data and flux observations to provide high resolution spatio-temporal GHG flux fields. Most important, the current data assimilation system approach, which up to now is only capable of using in-situ observations, needs a transition to a completely new ("integrated") system that uses synergies with national weather prediction, and that is capable of assimilating data from the wealth of observational capacities including ground based and space-borne remote sensing, (regular) aircraft measurements, and that delivers products compatible with the needs of users, e.g. sector specific and spatio-temporally resolved GHG emissions.

The overall outcome of the ITMS is planned to include:

a) online provision and visualization of natural and anthropogenic GHG sources and sinks for Germany, sector specific as well as adequately spatially resolved and temporally sampled
b) support to Monitoring, Reporting and Verification (MRV), especially the national inventory reports, and aiding scientific evidence for certificate trading
c) detecting over- and underestimation of sources and sinks, thereby reducing uncertainties w.r.t. sectorial attribution as well as spatio-temporal variability
d) regional hotspot characterization
e) differentiation of natural and anthropogenic contributions, and the quantification of diffuse sources and sinks of GHGs such as agriculture, forestry and other land use (AFOLU), but also traffic
f) integration of German observing and modelling capabilities to set up a national service, i.e., enabling the continuous use of Copernicus services, EU research projects, ICOS, IAGOS, as well as satellite data for advising society and policy

g) evaluation and improvement of observational strategies and support other countries for implementing GHG observation systems
h) target-oriented consultancy of industry and policy w.r.t. success of mitigation measures

Through the optimal bundling of the high-quality individual efforts on systematic observations, modelling and data assimilation within the German research community, the ITMS will strengthen Germany's position within the Global Environmental Change research landscape. This provides added value, makes it strategically independent and internationally competitive. Based on these strengths, ITMS will cooperate with international partners in research in the following areas:

- further development of the understanding of the relevant source and sink processes;
- improved spatial and temporal resolution of bottom-up descriptions of anthropogenic and biogenic sources and sinks;
- development of top-down model systems for the operational environment, including the interaction with global models;
- optimization of the use of in-situ (ground-based and airborne) and satellite based remote sensing data (Sentinel-5 Precursor (S5P), OCO-3, GOSAT-2, the French-German cooperation MERLIN and, in perspective, data of the Sentinel satellites S2, S5 and CO2M).

The vision is a system capable of combining and using the further increasing power of atmospheric observations from ground, air and from space, high spatio-temporal resolution bottom-up flux modelling, and high resolution atmospheric (inverse) modelling for monitoring and documenting GHG sources and sinks in high spatio-temporal resolution, thereby matching user requirements and allowing the implementation of an independent Monitoring, Reporting and Verification (MRV) system for GHG emissions from diffuse sources such as e.g. agricultural activities.

The scale of atmospheric observations, from point scale for in-situ measurements to the kilometre scale for remote sensing, combined with the spatial scales at which surface-atmosphere fluxes vary, requires atmospheric transport simulations at kilometre scale, and a corresponding resolution in prior fluxes, even if targeted products (i.e., top-down estimated GHG balances) might not be needed at such high resolution. The gradual development of including additional data streams, increasing resolution, introducing more comprehensive prior fluxes, and improving atmospheric transport modelling will be accompanied by a strong effort to continually monitor the performance of the system. In addition to uncertainty reduction, the system's capability to reproduce withheld data (cross-validation) will be used as a performance measure.

By using the findings and data of current and future EU programmes, these research foci are intertwined in many ways with the European research context: in particular with ICOS, Copernicus (CAMS, C3S, CO2M) and H2020 projects (CHE, VERIFY, CoCO2 and follow-up projects), both ecosystem- and atmosphere-focussed. It is also planned to link the ITMS results with the ICOS Carbon Portal (https://www.icos-cp.eu/). In contrast to the international activities, the ITMS research focuses on the national scale and below. It will result in an operational, state-of-the-art German ITMS, delivering sector specific high spatially and temporally resolved information on GHG sources and sinks, which is currently not existing.

2.2 Context within political research guidelines

The 2030 Agenda for Sustainable Development, adopted by all United Nations Member States in 2015, lists as its heart 17 Sustainable Development Goals (SDGs). The new FONA (Forschung für Nachhaltigkeit, or Research for Sustainability) strategy as formulated by the BMBF refers to these SDGs, specifically mentioning SDG 13 "Climate Action". The ITMS is intimately linked with this SDG, as it provides a basis for independent estimation of anthropogenic GHG emissions.

Within the Paris agreement (2015) the participating countries have agreed to implement a transparency framework for monitoring the impact of the Nationally Determined Contributions (NDCs) to the reduction of emissions of greenhouse gases (GHGs). The UNFCCC inventory reporting for Germany is provided by UBA. The Intergovernmental Panel on Climate Change (IPCC) and the United Nations Framework Convention on Climate Change (UNFCCC) recommend supplementing the national inventory reports (NIR) with activities for independent monitoring of greenhouse gas sources and sinks. Within the 2019 refinements of the 2006 IPCC guidelines for national greenhouse gas inventory reporting, it is suggested to consult inverse modelling products for quality control and verification of national emissions [2]. The World Meteorological Organisation (WMO) is developing the Integrated Global Greenhouse Gas Information System (IG3IS) framework, with recommendations for national contributions. The German contribution to WMO IG^{3}IS is the Integrated Greenhouse Gas Monitoring System (ITMS, "Integriertes Treibhausgas-Monitoringsystem").

2.3 Stakeholders and needs

The Paris Climate Agreement aims to reduce anthropogenic greenhouse gas (GHG) emissions by means of nationally determined contributions (NDCs) (UNFCCC, 2015). Therein it is foreseen that as of 2023 a Global Stocktake will take place **every 5 years** to assess the parties' progress made towards achieving their long-term goals. During the *Conference of Parties* COP24 (Katowice 2018) an *Enhanced Transparency Framework* was approved, stipulating *Biennial Transparency Reports* to be prepared **every 2 years** from 2024 onwards. In light of the growing request on GHG information and its uncertainties, the need to operate an integrated greenhouse gas monitoring system is indispensable for the foreseeable future. Article 4.3 of the Paris Agreement requires that each Party's successive NDC has to represent a progression beyond the Party's then current NDC and reflect its highest possible ambition, reflecting its respective capabilities.

On the national scale, the Bundes-Klimaschutzgesetz (KSG) [see, e.g., 3] was implemented on 18th December 2019 to ensure the international goals are met. In §3 KSG the mitigation goals are defined up to 2030, aiming at achieving GHG neutrality by 2050 (§1 KSG). The Federal Constitutional Court ruled on 24th March 2021 [4]: '*The statutory provisions on adjusting the reduction pathway for greenhouse gas emissions from 2031 onwards are not sufficient to ensure that the necessary transition to climate neutrality is achieved in time'.* Thus, in addition to the international agreements, national rule requires more detailed emission targets and transparency [5] to achieve climate neutrality by 2050. Net GHG neutrality is defined in KSG as balancing anthropogenic emissions with sinks. Clearly, the sources and sinks have to be objectively determined. While UBA collects the sector emissions (§5 KSG), it is the responsibility of the *Expertenrat für Klimafragen* (according to §12 Abs.1 KSG) to examine the process of emission data collection and its temporal change, as well as to recommend further actions. In the 2021 report of the *Expertenrat für Klimafragen* the options of independent verification are discussed in relation to IG3IS and the potential of the future ITMS for Germany [6, section 8.1, Abs. 180].

Supporting the *Expertenrat für Klimafragen* with information is an important ambition of ITMS. First results of ITMS will be communicated to this consultation group and other users and stakeholders (scientific institutions, governmental institutions – during this Demonstration Phase especially UBA, TI and DWD with their corresponding ministries), and climate science communication facilitating organisations like DKK (Deutsches Klima Konsortium), which regularly provide press releases and newsletters or social media information. Preliminary concepts for communication between ITMS and *Expertenrat für Klimafragen* will be investigated within the Demonstration Phase before 2024.

Important scientific stakeholders of ITMS are also in the international research community.

3. State of the art and ITMS phases

3.1 Research state of the art

Monitoring of GHG emissions became a focus of current research for more than a decade. For example, projects such as CarboEurope made the first attempt to combine observational data streams on atmospheric composition and inverse modelling approaches (so-called "top-down" constraint) with bottom-up information from emission inventories, process level studies, satellite imagery and flux models. The projects CHE (CO_2 Human Emissions) and VERIFY, currently followed by COCO2 (Prototype system for a Copernicus CO_2 service) are taking steps towards defining an operational observation-based system for monitoring and verification of greenhouse gases, targeting the European scale, with the aim to implement an operational system in the European Copernicus Services. CHE focussed on the development of an operational monitoring capacity for anthropogenic CO_2 emissions, the implementation of OSSEs (Observation System Simulation Experiments) to assess the requirements of an operational system, and the construction of a prototype system with a global/European spatial focus. VERIFY has a focus on emissions of CH_4 and N_2O as well as CO_2, including land use related sources and sinks, with a spatial focus on Europe. VERIFY will use existing observational datasets to further develop research inversion systems into a pre-operational system. The COCO2 project is building the prototype system for a European Monitoring and Verification Support capacity for CO_2 and CH_4. The provision of natural CO_2 sources and sinks utilizes the CarboScope Regional inversion system (CSR) developed at MPI-BGC [7], which will be further developed within the ITMS. VERIFY has a strong focus on establishing collaboration between research institutes and national inventory agencies, which for the German case provided a basis for collaboration with UBA. VERIFY takes first steps to combine Carbon Cycle Data Assimilation System (CCDAS), in which ecosystem model parameters are jointly optimised from land and atmospheric observations, with a Fossil Fuel Data Assimilation System (FFDAS) that utilizes a dynamical emission model within an atmospheric inversion framework.

The results and experiences from these three projects will be used for the national ITMS research project through the participation of several ITMS partners in CHE, VERIFY and COCO2, but cannot be directly transferred due to the different scales (European vs. national and sub-national for Germany). Within the framework of CAMS, daily forecasts of greenhouse gas concentrations are generated using satellite data assimilation for CO_2 and CH_4 (GOSAT) at a resolution of 9 km, but the assimilation optimizes atmospheric mixing ratios rather than underlying fluxes. The resulting high-resolution fields, together with in-situ observations are being used in global inversion calculations to estimate GHG fluxes at the relatively coarse resolution of several hundred kilometres.

Regarding observational data streams, there has been an effort in the development of systems to measure GHG emissions on city-scale within CarboCountCity, or temporarily with several spectrometers operated in the framework of the COCCON network [8] deployed around Paris [9] or Berlin [10]. For measuring the GHG emissions of Munich permanently, an autonomously operated array of COCCON spectrometer systems is under development [11]. Successful use of spectrometers from ground (COCCON) and aircraft (MAMAP) for quantifying XCH4 emissions from extraction of fossil energy sources or landfills have already been demonstrated [12,13]. By being close to anthropogenic emission hotspots, various local emission sources can be disentangled [14]. Those local observing systems are complementary to the remotely located ICOS stations [15], which were designed to understand the natural sinks and source processes. By using specific atmospheric indicators of fossil CO_2 combustion such as radiocarbon (^{14}C in CO_2) or CO, fossil CO_2 emissions can be separated from biogenic fluxes at European [16] and regional scale [17]. In addition, IAGOS was established to provide quasi-operational data on GHG and other gases along flight corridors from using civil aviation as infrastructure [18]. Another important pillar is the progress made on remote sensing of atmospheric GHG concentrations from satellite and from the ground. Especially satellite remote sensing has recently made an important step in providing methane distributions from the S5P mission globally with a spatial resolution allowing applications at and below the national scale. In addition, in an initial case study it was demonstrated that the combination of satellite XCO2 and trop. NO_2 allows to quantify anthropogenic CO_2 emissions from space [19]. In Europe satellite remote sensing of GHG will be further developed towards operational applications via the Copernicus CO_2 Monitoring Mission (CO2M) [20] conceptually initiated by Carbonsat mission [21], and the German-French MERLIN mission [22]. To establish the link between satellite and ground based GHG measurements, TCCON [23] was established, and recently supplemented by COCCON [8], as the reference network for ground-based observations of column-averaged GHG abundances.

With the ITMS initiative, all these scientific developments are used together and developed further into a common GHG monitoring system for Germany.

3.3 Implementation Phases of ITMS

The long-term vision of the ITMS is to serve as (1) an operational service providing input to policy advice and informing the general public on the effectiveness of GHG reduction (NDCs), and as (2) a research infrastructure which enables collaboration with the scientific community to work on relevant research questions, such as identifying hot-spots of emissions, targeting of most promising mitigation regions, unravelling feedback mechanisms between climate change and natural fluxes, or research on “tipping points”, encouraging input from the community for on-going development of the infrastructure.

This requires careful planning regarding the construction and early deployment phase of the infrastructure to arrive at operational readiness while establishing and fostering collaboration with the scientific community. The planning also needs alignment with external activities like the global stocktake.

The planning involves three phases (see Fig. 2): Phase 1 is a development phase providing a demonstrator ITMS, Phase 2 aims at establishing a first-generation ITMS capable of providing regular information on GHG emissions based on numerous observational data streams, and Phase 3 is concerned with the transition to a fully operational system at DWD.

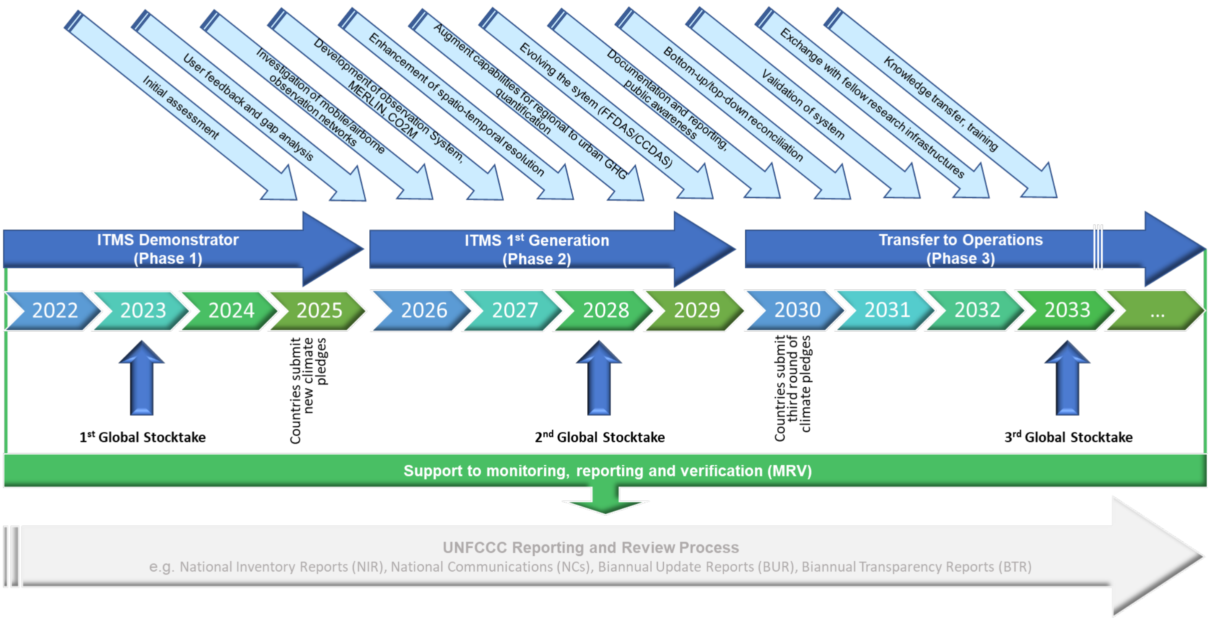

Figure 2: The longer term perspective on the ITMS development: Phase 1 (ITMS Demonstrator), Phase 2 (ITMS First Generation) and Phase 3 (Transfer to operations). In order to demonstrate the timeliness of the ITMS development is has been put into context with the UNFCCC reporting and Review process for which UBA is in charge at national level. The pre-operational emission verifications are to be timed to match with the UBA reporting. It is expected that both quality and timing will get increasingly useful during the ITMS development. In order to optimally develop the system through phases 2 and 3 it is anticipated that at least the actions indicated by the light blue arrows have to be implemented in due course, as described in Chapter 2.5.

The **first ITMS phase**, described in the following sections in detail, comprises

i. the development of quality controlled observational data streams tailored to ITMS needs (Modules on Observations, named ITMS-B);

ii. the introduction of the assimilation of ground- and satellite-based GHG observations into modelling systems used at the DWD for weather forecasting and the provision of regular updated top-down estimation of natural CO_2 and anthropogenic CH_4 emissions using the pre-existing CarboScope-Regional inversion (within the Module on Atmospheric Modelling & Inverse Methods, named ITMS-M);
iii. establishing the provision of bottom-up GHG fluxes at high spatio-temporal resolution using empirical, semi-empirical and process-oriented modelling approaches (Modules on Sources and Sinks , named ITMS-Q&S).

During this phase, also a closer link between bottom-up flux estimation from module ITMS-Q&S as a-priori fluxes and the top-down estimation is developed by means of high spatio-temporal resolution and full error characterisation of the prior flux fields. This phase will assess to what extent ITMS is able to distinguish between sectorial emissions and to provide input to the Global Stocktake of 2023 and future stocktakes.

During the **second ITMS phase**, it is envisioned to introduce massive remote sensing data streams into the GHG data assimilation system to constrain GHG emissions further, which will finally also allow to improve the predicting capability of bottom-up modelling approaches. With novel GHG observations from space, as provided by OCO-3 and S5P, S5 and as expected during phase two with higher spatial resolution from the Copernicus anthropogenic CO_2 Monitoring (CO2M) satellites and from MERLIN (CH_4), current inverse modelling approaches will reach their limit due to the sheer number and density of such observations and due to their spatial representativeness. The CarboScope-Regional inversion system will serve as a reference tool for the GHG data assimilation system. During this phase, also regular reporting of top-down constrained N_2O emissions will be developed. An even stronger link between bottom-up modelling approaches and the top-down data assimilation is envisioned by moving from determining corrections to prior fluxes to determining key geophysical and human activity parameters controlling the fluxes using dedicated flux models. This phase is envisaged to inform on sectoral emissions and provide input to national reports as well as the global stocktake 2028.

Phase three is anticipated to be dedicated to the transition to a routine operational service at DWD. This will require further research to validate and evolve the system. It is envisioned that by then the operational tools can be used to address upcoming research questions in the area of GHG emissions.

4. Structure and time line of Phase 1

The required Phase 1 work is organized in **seven modules** (see Fig. 3):

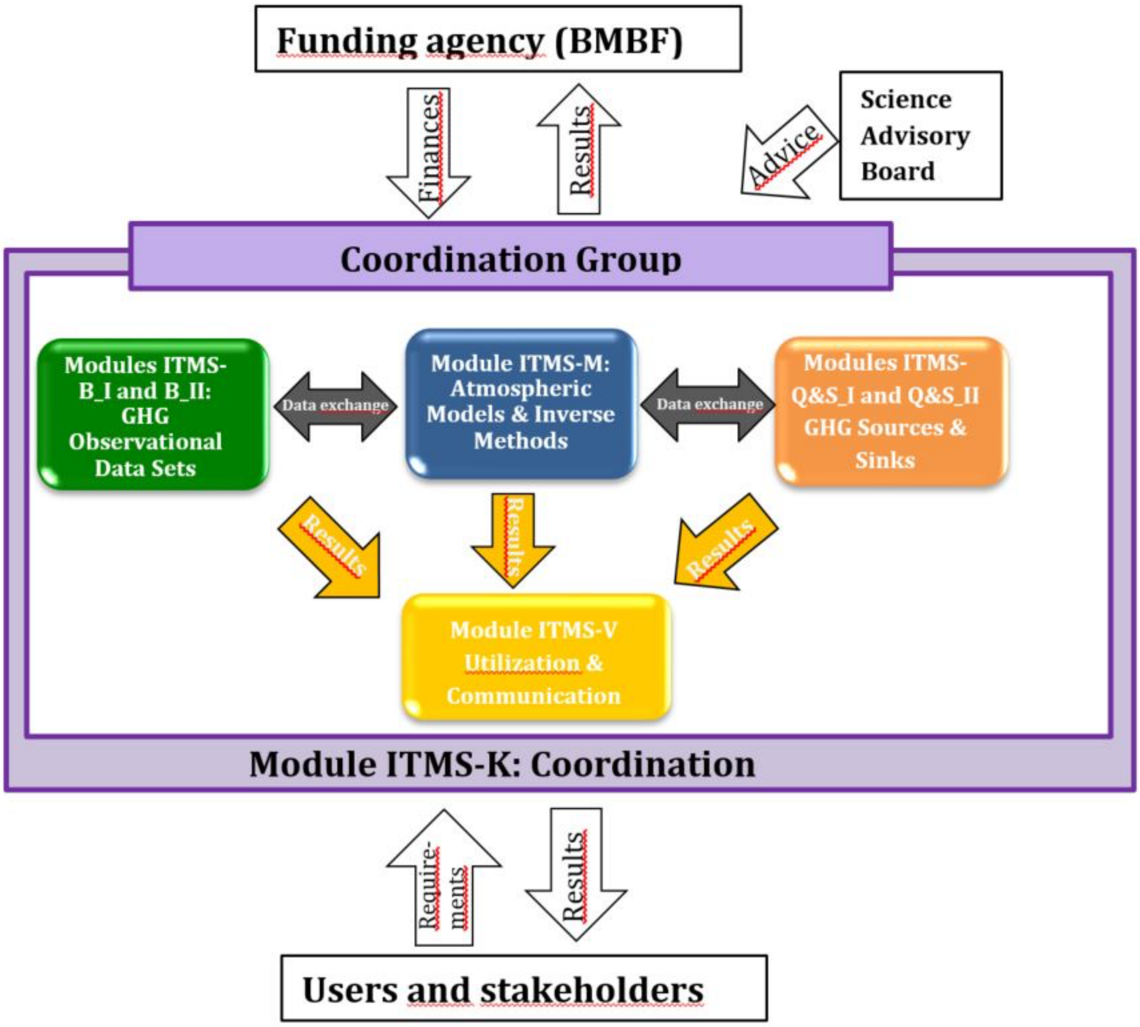

Figure 3: The goals of the operational ITMS are aligned to serve the needs of users and stakeholders. For this, the ITMS project will perform research & development, exchange of data and scientific results (grey arrows) and stepwise transfer to operations (yellow arrows).

Module K ("Koordinierung", Coordination)

is in charge of coordination, overall operations of ITMS and management.

Module V ("Verwertung und Vermittlung", Utilization and Communication)

integrates users and provides consistent communication including visualization of results, as well as coordinates the contributions substantiating the national GHG reporting.

Module M ("Modellierung", Atmospheric Models & Inverse Methods)

develops atmospheric & inversion models linking the concentration data (Modules B) with the surface flux parameterizations (Modules Q&S), to develop a prototype ITMS.

Modules B ("Beobachtung", Greenhouse gas observational data sets for ITMS)

develop and secure data flows and quality of atmospheric GHG observations (in-situ and column concentration data) as input for the data assimilation and flux data for model verification. The data flow is building upon data from available observational infrastructure from e.g., ICOS, IAGOS, TERENO, ACTRIS, TCCON, COCCON and the data products retrieved from different satellite borne instrumentation (e.g. S5P, OCO-3, GOSAT-2, S-5, MERLIN, CO2M, MODIS, VIIRS, S-2/-3). In addition, research on new observational approaches will be performed with the goal to close observational gaps. Modules B work is implemented in B_I and B_II:

Module B_I contains core work packages of Modules B

Module B_II contains "called" work packages of Modules B

Modules Q&S („Quellen & Senken", Sources and Sinks of Greenhouse Gases), provide bottom-up quantification of sources and sinks, parameterising of process/ecosystem- fluxes and anthropogenic emissions of GHGs from local to regional scales such that they can be used as "*a-priori*" or "*prior*" fluxes in the other Modules. The Modules develops model approaches which allow to simulate the surface-atmosphere exchange of GHG in high spatio-temporal resolution, together with a thorough assessment and communication of uncertainties. Modules Q&S work is implemented in Q&S_I and Q&S_II:

Module Q&S_I contains core work packages of Modules Q&S

Module Q&S_II contains "called" work packages of Modules Q&S

As the ITMS modules have both English and German module names and abbreviation in different documents, Table 1 provides a detailed explanation.

Table 1: Summary of ITMS Module name and acronym definitions

Verbundvorhabensbeschreibung		**Acronym**	**Content**
English name	**German name**		
ITMS-COORDINATION	ITMS-KOORDINATION	ITMS-K	Coordination of the overall ITMS-Project across all modules
ITMS-MODELLING	ITMS-MODELLIERUNG	ITMS-M	Atmospheric Models & Inverse Methods
ITMS-OBSERVATION_I	ITMS-BEOBACHTUNG_I	ITMS-B_I	Core greenhouse gas observational data sets
ITMS-OBSERVATION_II	ITMS-BEOBACHTUNG_II	ITMS-B_II	Called greenhouse gas observational data sets
ITMS-SOURCES&SINKS_I	ITMS-QUELLEN&SENKEN_I	ITMS-Q&S_I	Core sources and sinks of greenhouse gases
ITMS-SOURCES&SINKS_II	ITMS-QUELLEN&SENKEN_II	ITMS-Q&S_II	Called sources and sinks of greenhouse gases
ITMS-UTILIZATION& COMMUNICATION	ITMS-VERWERTUNG und VERMITTLUNG	ITMS-V	Utilization and communication of ITMS results

4.1 Overall schedule of ramping up the Demonstration Phase

A stepwise start of the work is planned for the ITMS project. It is useful that selected Workpackages of Module M start in 2021 a few months ahead, to prepare an efficient ramp up of ITMS-M in 2022 which builds the foundations for a pre-prototype for operational ITMS together with ITMS-B_I and ITMS_Q&S_I. The call for ITMS-B_II and ITMS- Q&S_II contributions will augment the consortium with more partners, their contributions improving the zero version by means of introducing more or better data, and developing methods increasingly fitter for purpose.

The project contributions acquired by the call are expected to start in 2023, one year after the first work of the core parts will have started.

Two years after the start of the core consortium Module V will start utilization and communication of results.

Table 2: Timing of ITMS modules in Phase 1

	2021	2022		2023		2024		2025	2026
ITMS timescale	1	2-3	4-13	14-15	16-25	26-27	28-37	38-49	50-51
ITMS-M									
ITMS-K									
ITMS-B_I									
ITMS-Q&S_I									
ITMS-B_II									
ITMS-Q&S_II									
ITMS-V									

The ITMS modules work together to achieve the overall ITMS aims. The individual work plans of all modules are overseen by ITMS-K to coordinate interaction and timing of deliverables between the different work packages.

4.2 Project organization and responsibilities

Following management structure is planned for the ITMS:

Steering Group: The Steering Group is the decision-making body of the ITMS project. It comprises the body responsible for the project (*Projektträger*), the Coordination Group and important invited stakeholders as ministries and subordinate agencies. The Steering Group meets at least once per year, preferably connected to the annual general meetings, and additionally as needed.

Coordination Group: The Coordination group is overseeing the progress of the ITMS project at the management and scientific level. It takes scientific advice from the external Science Advisory Board and discusses status and development of ITMS in the General Meeting. It decides on its composition and has at least the project coordinators and the module coordinators as members. The coordination group meets monthly in virtual meetings and according to needs. As of 2021, the coordination group consists of following members: Dr. Christoph Gerbig (MPI-BGC Jena), Dr. Andrea Kaiser-Weiss (DWD), Dr. Heinrich Bovensmann (University of Bremen), Prof. Dr. Klaus Butterbach-Bahl (KIT-IMK-IFU), Dr. Christian Plaß-Dülmer (DWD) and Dr. Andreas Fix (DLR).

Project Coordinators: The ITMS project coordinators Dr. Christoph Gerbig (MPI-BGC) and Dr. Andrea Kaiser-Weiss (DWD) are jointly heading the coordination group. The project coordinators represent the project to the funding agency and outside of ITMS.

Module Coordinators: The Module coordinators organize collaboration in their respective Modules, ensuring that Milestones and Deliverables and communication with the other modules are in time and appropriate to achieve the objectives

Scientific Advisory Board: An external Scientific Advisory Board will be established comprising 3-5 members recruited from international experts. The Scientific Advisory Board will be formed during the project start phase. Members are selected with respect to scientific merit in corresponding scientific areas and connection with potential users.

General Meeting: The General Meeting (GM) consists of all partners and is the forum for data and knowledge exchange and for discussion of any issue concerning the proper operation of the consortium, the compliance with work plans and the discussion of benchmarking and of planning for next project phases. Members of the Scientific Advisory Board are invited to the GM. The GM is invited and chaired by the project coordinators. The General Meeting is organized once per year.

All aspects of project management are performed in module ITMS-K. Utilization and dissemination of results are performed in Module V, with the involvement of the Coordination Group and module ITMS-K.

Agency users expected to benefit significantly from the ITMS results are involved from the start of the project. Intensive user and stakeholder interaction is foreseen to capture user requirements and provide corresponding products.

4.3 Meetings and conferences

Kick-off meetings are planned when major scientific work contributions start, focussing on the presentation and elaboration of objectives, state-of-the-art, challenges, task-planning, Milestone-structure and cooperation between Workpackages.

Benchmark meetings, matched with the Milestone time plan, focus on progress of the project, critical issues, lessons-learned, and planning for next steps/phase. For interfacing of all ITMS Modules, annual General Meetings (GM) are planned, with break-out meetings for individual ITMS modules. The organization of the meetings is task of the module ITMS-K, WP 1.

General Meetings are held once a year to facilitate collaboration, inform about progress and resolve issues.

Module specific meetings are in the responsibility of the respective modules and are planned as required. ITMS-K for instance has monthly virtual meetings, but beside the Kick-off and Benchmark meetings and GMs no independent physical meetings are planned.

Working meetings between selected partners are held when this is the most efficient way to proceed, the planning is also in the responsibility of the respective modules.

4.4 Milestones

The interaction between the ITMS Modules concerns fitting data streams and information feedback loops between the Modules, and a matching of time and space scales with the inherent variabilities and uncertainties. This requires an effective collaboration and linkage between the project activities. An effective cooperation will be facilitated by Module ITMS-K and structured according to a hierarchy of specific Milestones of the overall ITMS project, Milestones in the Modules ITMS-M, ITMS-B_I and ITMS_B_II, ITMS-Q&S_I and ITMS-Q&S_II, and Deliverables specified in the individual work-packages (Fig. 4).

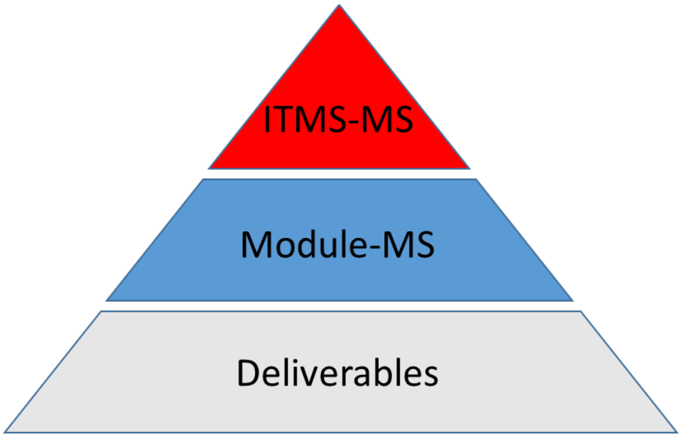

Figure 4: Hierarchy of the overarching Milestones (MS) of ITMS, the next level of the Module related MS, and the mostly WP related Deliverables.

The Milestones (MS) describe specific achievement of the Modules and the whole project and thus are central in controlling the success of ITMS. All WPs describe their contributions to specific MS and thus their role in achieving the objectives of ITMS. Module ITMS-M is the central Module of ITMS in developing an operational inversion system of GHG and allowing the monitoring of GHG according to the specified objectives (see above). Thus, MS in Modules ITMS-B and ITMS-Q&S are supporting MS in Module ITMS-M and the overarching MS of ITMS. A flow diagram illustrating the MS and some of their substantial interaction is shown in Fig. 5, details and more comprehensive explanations are given in the respective module descriptions.

Fostering an optimal interplay between the ITMS project Modules, overall progress can be measured with overall Milestones, as the progress of all Modules effort are transferred together into measureable results there, see Table 5 and Fig. 5 below.

Table 5: Overall ITMS Milestones

ITMS-MS	Milestone name	Responsible	ITMS project month
ITMS-MS1	First CH4 and B-CO2 inversions	MPI-BGC	22
ITMS-MS2	Second CH4 and CO2 inversions	DWD	34
ITMS-MS3	Status review and planning of Phase 2	MPI-BGC	38
ITMS-MS4	Third CH4 and CO2 inversions	DWD	46
ITMS-MS5	Achievements, final Reporting	DWD	51

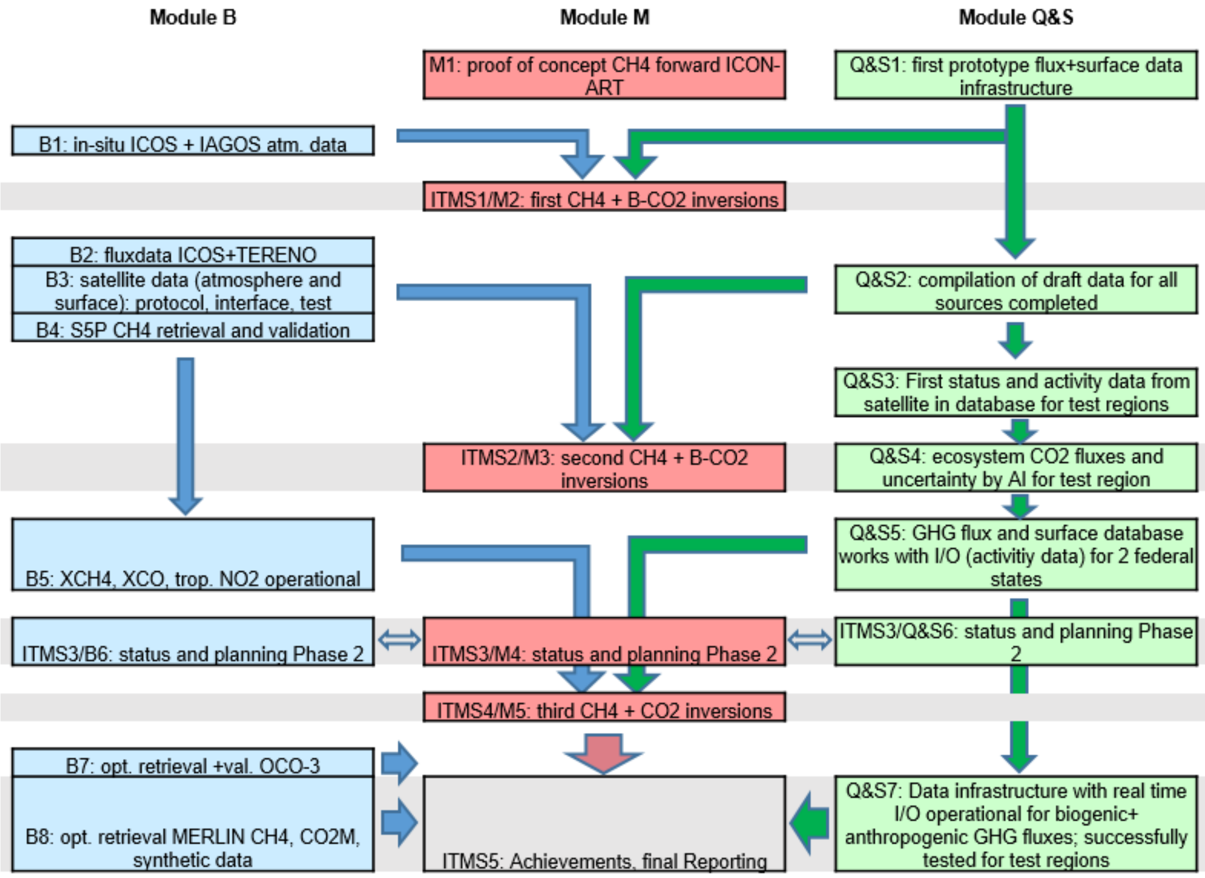

Figure 5: Flow-diagram of the Milestones (MS) in the central Modules of ITMS. Overarching Milestones are named as ITMS1-5. the Module specific MS follow the nomenclature B/M/Q&S1-8. Arrows indicate relations to other MS. The success of the ITMS project will be controlled by achieving the Deliverables and Milestones. Accordingly, cooperation between partners, communication and meetings with associated schedules and participants are organized around these MS. Risk analyses refers to achieving specified Milestones.

The five overarching Milestones ITMS.1-5 (see Fig. 5) serve as top-level indicators for the success of the developments during the Demonstration Phase of ITMS.

5. Project Phase 1 (Demonstration Phase) Work Plan per Module

5.1 Module M: Atmospheric Models & Inverse Methods

ITMS-M will research the basics of a modern system for GHG emission monitoring and prepare the long-term uptake and utilisation of ITMS results into operational services. As the German weather service (DWD) has a permanently working operational environment for data handling, data assimilation and forecasting in the context of operational weather forecasting and reanalysis, as well as climate data curation, it is a natural choice to establish the long-term capability for GHG data assimilation there. Also, DWD is responsible for atmospheric observations of greenhouse gases in the ICOS framework. Thus, the connection of ITMS-M developments in connection with the operational systems of DWD allows for making full use of existing synergies. ITMS-M will regularly provide top-down estimation of GHG exchange, starting with CH_4 and natural CO_2 exchange fluxes, and advancing with the input of the Module ITMS-Q&S to full CO_2 fluxes (natural and anthropogenic), and will provide sectorial and spatial information on emissions employing observations from Module ITMS-B during Phase 1. This information will be used to augment the annual national inventory reports, i.e. ITMS based results will be added as a supplement to the NIR.

The aim of this research is to combine relevant experiences at the different institutions (DWD, KIT-IMK-ASF, MPI-BGC, and UHEI), and develop the elements of a data assimilation system that is capable of using information from a variety of data streams, including ICOS, IAGOS, TCCON and (imaging) satellite instruments. The work is divided into 13 Workpackages (WPs), with phased starting times fitted to the needs, each with one or two researchers performing the work in collaboration.

One of the challenges is the requirement to provide continued updates of top-down constrained GHG fluxes, while in parallel developing a GHG data assimilation system using ICON-ART. This will be met by using the existing CSR inversion system as an interim tool (WP-M.2), in which also various developments (improvements in vertical mixing, utilization of full profile data from ICOS and IAGOS) can be tested (WP-M.3 - WP-M.6). The ICON-ART based GHG data assimilation system will be developed up to a demonstrator stage with benefit expected from the collaboration with MPI-BGC Jena w.r.t. flux inversions, such that in the subsequent phase GHG flux estimates can be provided by the ICON system.

Weather forecasting is an initial value problem, with assimilation cycles using observations over short time windows (usually a few hours) to derive an analysis (the best guess for the atmospheric state at the start of the forecast, or the initial value). DWD employs for its ICON model a hybrid data assimilation method. It consists of an ensemble Kalman filter (EnKF) coupled with a three-dimensional variational analysis (3D-Var). The ensemble Kalman filter uses an ensemble of states to estimate the uncertainty, the three-dimensional variational analysis retrieves an optimal estimate of the atmospheric state. To make such a system useable for estimating surface-atmosphere fluxes of long-lived tracers, atmospheric tracer observations need to be used over a longer assimilation cycle, as the link between surface-atmosphere fluxes and tracer concentration is not instantaneous, but acts over timescales of atmospheric transport (advection and mixing). The basic idea is to use a similar data assimilation system, but using ensemble members with different prior flux error realizations rather than different initial conditions, such that the ensemble represents the full a-priori knowledge about GHG fluxes. We will assess synergies in the development of ensemble-based simulations with CIF, the Community Inversion Framework (http://community-inversion.eu), under development within the H2020 project VERIFY.

The adaptation of the modelling and data assimilation currently used at the DWD for weather forecasting to a system assimilating GHG observations will be done in several steps: forward modelling (WP-M.7), assimilation of point observations (WP-M.8), then satellite data (WP-M.9), to obtain an improved spatio-temporal atmospheric distributions of GHG concentrations (still very similar to NWP), and finally ensemble simulations of GHGs combined with Kalman filtering (WP-M.10).

A further challenge is the need for an on-going check of the system's performance, while continuously new developments are being implemented. This challenge will be met by setting aside specific parts of the data streams (atmospheric data, bottom-up estimates of fluxes) and assessing the performance of the system by comparing optimized fluxes and atmospheric concentrations with these data streams in a quantitative way, including the posterior uncertainties. This way, the uncertainty reductions calculated formally within the system will continually be evaluated, and improvements in skill of the GHG assimilation can be assessed. These withheld data will also include data from dedicated regional campaigns such as proposed within the ITMS.

The individual Workpackages are briefly explained below. Note that many Workpackages will require input from the collaborative projects ITMS-Observations and ITMS-Sources&Sinks (indicated below as Module B, or WP-B.*, Module Q&S, or WP-Q&S.*), with fall-back options in case of delay identified. Within the overall ITMS coordination (collaborative project ITMS-Coordination) the timely availability of those required products will be ensured. Furthermore, results from several Workpackages are communicated to users through project ITMS-V (Utilization and Communication).

WP-M.1 Consolidation of experience

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

Participating partner: MPI-BGC, Dr. habil. Christoph Gerbig

The existing experiences with existing data assimilation with ICON and ICON-ART are combined with the experiences with flux inversions from the CarboScope Regional inversion system (CSR). Other research, e.g. with WRF-GHG and from the Copernicus services are included in the review.

WP-M.2 Evaluation of biogenic CO2 fluxes and anthropogenic CH4 emissions

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

To continuously provide information to be used as annex to the national GHG reporting, the existing CSR inversion system will be used initially for CH_4. As biogenic CO_2 fluxes from biospheric photosynthesis and respiration processes in Germany are larger than the anthropogenic emissions, and are subject to larger uncertainties, at this stage anthropogenic fluxes of CO_2 are prescribed in the inversion. With the use of CAMS boundary conditions and ICOS data, a near-real-time inversion system is to be set up to provide sub-annual updates of GHG flux estimates. Should bias errors in CAMS GHG fields still prevent this, the global CarboScope model will be used to provide boundary conditions. Atmospheric observations provided by Module B, covering year n-1, will be used in the flux estimate that will be delivered around September of year n. The system will be continuously updated.

WP-M.3 Implementation of ICON meteorological fields in CSR

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

The CSR system uses the Lagrangian model STILT driven by meteorological fields (winds etc.) from the ECMWF IFS at a resolution of 0.25° × 0.25° (roughly consistent with the spatial resolution of IFS fields in 2006). The NWP system at DWD can provide met. fields from the ICON-EU nest at a much higher resolution (6.5 km). To improve on the Lagrangian transport these meteorological fields shall be implemented for use within STILT. This also enhances the comparability with the ICON-ART based GHG data assimilation when the CSR is used as a reference inversion.

WP-M.4 Improvement of vertical mixing

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

Participating partner: DWD, Dr. Linda Schlemmer

A significant limitation in inverse transport modelling of sources and sinks of greenhouse gases results from the necessary parameterisation of unresolved mixing processes (turbulence) in the atmospheric boundary layer, which leads to an inaccuracy of the vertical profiles of GHGs and in an inexact estimate of the height of the mixing layer (mixing height MH). Observation-based MHs can be derived from radio soundings (weather balloons), aircraft data (AMDAR), and from ceilometers or lidars.

So far, simulated MHs have been compared with observations from radiosondes, and, using Kriging interpolation to combine simulated and observed MHs, improved STILT simulations of atmospheric transport have been possible [24].

Within this WP, the massive data stream from the Ceilometer Network of the DWD with more than 150 stations will be used to derive MHs. In the STILT approach, those will be used to obtain optimized MH fields for use in STILT and thus in CSR inversions.

In the ICON approach, different MH definitions will be evaluated using observations. This will be done offline using output from ICON simulations. The most promising approaches will be implemented into the ICON model in order to compute MH online on the native ICON grid. Moreover, the distribution of GHGs within the mixed layer and MH will be used to further evaluate the PBL parameterization and its interplay with the shallow and deep convection scheme in ICON-ART. By comparing to observations, the modelling settings best suited for the greenhouse gas concentration modelling in 3D and time evolution as needed for the ITMS emission verification will be identified.

WP-M.5 Utilization of ICOS and IAGOS vertical profiles

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

The current CSR inversion system only uses concentrations measured at the top level of ICOS tall towers, and only during conditions when the boundary layer is well mixed (i.e. 11:00-16:00 LT). ICOS profile data from the tall towers principally contain valuable information on nocturnal fluxes from the temporal change of the profile during (e.g. CO_2 increase as respired CO2 accumulates in the nocturnal stable boundary layer). Furthermore, IAGOS GHG data measured from commercial airliners provide high vertical resolution profiles up to and beyond the boundary layer, thus containing information on surface-atmosphere fluxes. This WP augments the CSR inversion system to utilize both these data streams.

WP-M.6 Simultaneous use of multiple species

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

The utilization of data streams of several greenhouse gases and associated trace gases in inverse modelling is expected to increase the reliability of estimated flux distributions through synergy effects. Those synergy effects result from similarities in emission patterns and in atmospheric transport for the different tracers. Prominent examples are the combination of atmospheric observations of CO2 and 14C-CO2 that allows for separation of biogenic from anthropogenic fluxes of CO2, and the use of Radon, which provides useful information on atmospheric mixing. Within this task, the capability to simultaneously assimilate observations of multiple species will be developed.

WP-M.7 Specification of the ICON forward model for ITMS

Responsible partner: KIT-IMK-ASF, Dr. Roland Ruhnke

DWD’s nonhydrostatic model system ICON (ICOsahedral Nonhydrostatic) is an online-coupled global to regional-scale modelling framework. The included Module ICON-ART (Aerosol and Reactive Trace gases) is designed for the simulation of the spatio-temporal evolution of aerosols and trace gases. ICON-ART-LAM is the limited area mode implementation, e.g., for Europe or Germany, which can be driven by external, e.g., CAMS concentration fields for trace gases at the boundary. Although GHGs have a long lifetime, for long-term monitoring purposes the chemical depletion has to be taken into account. For this, an altitude-spatial dependent lifetime-based approach being computationally cheap will be used via ART. In addition, by tagging the trace substances by source type (anthropogenic, biogenic) and source region, the contributions of individual source groups and regions can be distinguished and quantified. Extensive tagging allows for both sectorial disaggregation as well as separating emissions regionally. GHGs, passive tracers, and experiments with boundary conditions from Copernicus varying the grid and simulated model area, which are oriented on the operational NWP grids ICON-EU and ICON-D2, respectively, will allow to identify the optimal model setup. Performance optimization of the model system with respect to maximizing tagging capabilities as well as specification of number of affordable tags, grid resolution and model area is required in view of sensible computing power allocation and value added.

Experiments will be done with both ICON meteorology and CAMS meteorology as the boundary. Experiments will be repeated with increasing quality of Module Q&S a-priori fields. The quality can be accessed by comparing the forecasted concentrations with ICOS observations.

WP-M.8 Development of initial GHG assimilation within ICON-ART

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

The aim is to develop a demonstrator for assimilating the CH_4, CO_2 observations (preparing also for N2O) from ICOS or comparable point observations in the ICON-ART-LAM system by adjusting concentration fields. Synergies with the meteorological data assimilation environment at DWD are to be used, as this is the key for successful operations of ITMS in the future.

WP-M.9 Development of the ICON GHG satellite data assimilation

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

The initial GHG satellite data assimilation system within ICON-ART-LAM is developed, starting with CH_4 satellite column assimilation of S5P data, preparing for MERLIN CH_4 observations and CO_2 satellite observations. The assimilation will provide optimized concentration fields.

WP-M.10 Development of the ICON-ART GHG inversion for flux estimation

Responsible partner: DWD, Prof. Roland Potthast

This Workpackage develops the initial ICON GHG inversion system with ICON-ART-LAM, preparing for delivery of a posteriori emission estimates. The system should use strong synergies with the meteorological data assimilation environment at DWD, as this is the key for successful operations of ITMS in future.

The atmospheric data assimilation of DWD employs both variational and ensemble data assimilation techniques. On the global scale, the ensemble-variational method EnVAR for the deterministic global ICON model is used. A global ensemble data assimilation is based on the localized ensemble transform Kalman filter LETKF, also creating initial conditions for the ICON ensemble prediction system. On the convective regional scale, for COSMO-D2 the 4D-LETKF is run operationally for COSMO-D2 and COSMO-D2-EPS. For ICON-ART, in cooperation with Karlsruhe Institute of Technology (KIT), DWD is currently developing an EnVAR based data assimilation based on aerosol optical depth (AOD) retrieved from MODIS satellite measurements to assimilation measurements relevant to Saharan dust and volcanic ash.

The development of the data assimilation for the “Integrated Greenhouse Gas Monitoring System” ITMS intends to rely on the experience of the operational atmospheric and aerosol related assimilation systems, using as far as possible synergies with the CSR inversion scheme and also from the Community Inversion Framework (CIF) of H2020 project VERIFY.

WP-M.11 Transfer to operations

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

To prepare the future operational ITMS service, the operational environment for the ICON GHG emission inversion system is built and gradually optimized with respect to computing resources. The (intermediate) results of WP-M.7, WP-M.8, WP-M.9, and WP-M.10 are implemented and linked. Performance measures, also relying on independent data, are implemented. Computing performance is monitored. The system should especially focus on using strong synergies with the operational environment at DWD.

WP-M.12 OSSE for a urban scale observing system for anthropogenic CO_2

Responsible partner: UHEI, Dr. Sanam Vardag

Metropolitan areas and individual cities are committed, so-called "non-state actors" in the Paris Climate Convention; they are organized in initiatives such as C40 or ICLEI. Especially for these cities, significant changes in fossil fuel CO_2 (ffCO2) emissions are to be expected in the future. $^{14}CO_2$ is the most direct tracer for observing the CO2ff concentration. The current ICOS class-1 atmosphere station network provides the background activity of $^{14}CO_2$ for Germany and Europe, but it is not suitable for targeted monitoring of urban areas, as the ICOS stations explicitly avoid local anthropogenic source influences. Thus, in order to track CO2ff, additional observation networks adapted to the respective urban area are required.

The aim of this WP is to design cost-effective observation strategies for fossil CO_2 emissions from German cities and metropolitan areas. In the proposed observing system simulation experiment (OSSE), the potential of different observation networks and sampling strategies to quantify CO2ff emissions and reduce uncertainty will be investigated and evaluated. This will be done by high-resolution inversion of realistic synthetic concentration data including a-priori errors and model data mismatch. The EU-funded projects CHE and RINGO are currently pursuing similar questions, but on a European scale and with relatively low spatial resolution, or as case studies, e.g. for Northern France and the Benelux countries. The model study proposed here should concentrate on German conurbations such as Berlin-Brandenburg, Rhine-Ruhr area, Rhine-Main-Neckar area, as well as Munich and Nuremberg. The results of this model study provide the basis for an efficient and cost-optimised future CO2ff observation network of conurbations in Germany.

WP-M.13 Data management and stewardship of operational data streams

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

Main tasks are the quality monitoring and further development of the measurement data streams operationally required in the ITMS, the organisation of the operational interfaces and data flow of the auxiliary quantities, the troubleshooting and support of related Module B and Module M activities, the management of disk space and computer resources as well as quality assurance incl. version control, traceable documentation and archiving of the underlying material. Critical issues from an operational perspective are analysed and improved.

5.2 Modules B: GHG Observational Data Sets

Quality controlled observational data describing atmospheric greenhouse gas concentrations and fluxes are required to estimate top-down independent natural and anthropogenic greenhouse gas fluxes, to monitor the burden of greenhouse gases in the atmosphere, to validate transport and transformation mechanism in carbon models as well as to understand greenhouse gas exchange processes between the surface and the atmosphere in detail.

Modules B (“Beobachtung”, Greenhouse gas observational data sets for ITMS) develop and secure data flows and quality of atmospheric GHG observations (in-situ and column concentration data) as an input for the data assimilation and flux data for model verification. The data flow is building upon data from available observational infrastructure from e.g., ICOS, IAGOS, ACTRIS and TERENO as well dedicated data products retrieved from different satellite borne instrumentation (e.g. S5P, OCO-3, GOSAT-2, MERLIN, CO2M, MODIS, VIIRS, S-2/-3). In addition, in cooperation with other ITMS modules observational gaps will be identified and work will be stimulated to close observational gaps.

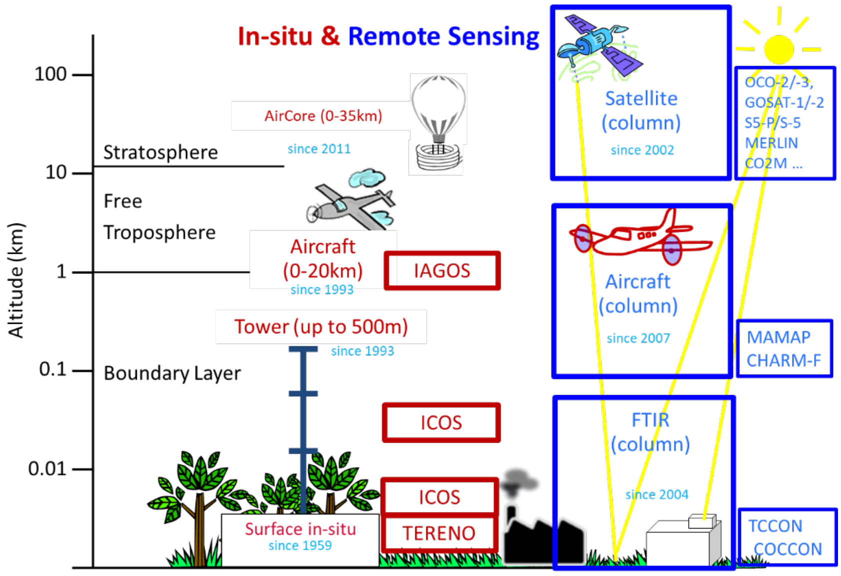

Figure 6: Atmospheric GHG observation system components contributing to ITMS. In addition, satellite data on vegetated surface properties will be included in ITMS.

During the last decade the German scientific community has led the progress in advancing the systematic observation of GHG gases through focussed field experiments and regular and operational observations utilising ground, aircraft, and satellite platforms. One prominent example is the German contribution to the WMO/GAW network and the European Integrated Carbon Observation System Research Infrastructure (ICOS RI). It now comprises operational observation networks (atmosphere, ecosystems and oceans) and central facilities. One major component of ICOS is the atmospheric observation network [15] with the continuous monitoring of atmospheric greenhouse gas (GHG) concentrations (CO_2, CH_4 and N_2O) combined with flask samples for their isotopic composition, radiocarbon sampling and tracer measurements (CO and ^{222}Rn) from a network of 12 stations, including tall towers, distributed over Germany. Continuous measurements of GHG fluxes (H_2O, CO_2) between different ecosystems and the atmosphere are carried out in the ecosystem observation network by the use of the eddy covariance technique.

The flux stations are arranged in clusters with different ecosystems being exposed to similar climatic conditions. In addition, measurements of GHG concentrations in the surface water and air-sea fluxes are carried out in the ocean observation network covering the North Atlantic Ocean and Baltic Sea. The resultant ground-based in-situ data sets are complemented on the global scale by the In-service Aircraft for a Global Observing System (IAGOS). IAGOS is a European Research Infrastructure for global observations of atmospheric composition from commercial aircraft [18]. IAGOS provides height-resolved in-situ data of greenhouse (CO_2, CH_4, partly N_2O) as well as reactive gases (O_3, CO, NO_x, NO_y) along flight corridors. In parallel to the progress made in operationalising ground- and aircraft-based in-situ measurements, the German remote sensing community made ground-breaking progress in achieving high precision total column concentration data on CO_2 and CH_4 from satellites (SCIAMACHY, OCO-2, GOSAT, S5P) and contributes significantly to the CEOS white paper on monitoring greenhouse gases from space [25], aircraft (MAMAP [26], CHARM-F [27]) and ground (TCCON [23], COCCON [8]). This paves the way for operational provision of CO_2, CH_4, CO and trop. NO_2 from satellite especially by Sentinel-5P (since Oct 2017) [28], Sentinel-5 (2024) [29], MERLIN (2027) [22] and CO2M (2026) [20] global data sets, with leading contribution from the German remote sensing community. These more operational oriented observation capabilities are complemented in Germany by innovative ground-based and aircraft in-situ and remote sensing campaigns. All these observational techniques have their strength and weaknesses. ICOS delivers temporally continuous in-situ concentration data of CO_2, CH_4 and N_2O with high accuracy and precision, but spatially sparse with low spatial resolution determined by their sampling footprint, IAGOS delivers high-quality concentration profiles of CO_2, CH_4 but is limited to major international airports and flight corridors. Satellite remote sensing provides globally consistent measurements of the dry atmospheric columns of CH_4 and CO_2, XCH_4 and XCO_2, having good spatial coverage and continuously improving spatial resolution (S5P XCH_4 and XCO with 7x 7 km2, CO2M XCO_2 and XCH_4 with 2x2 km2) but less precise than the local in-situ data. TCCON stations validates the satellite observations of XCO_2 and XCH_4 and establish the link between those observations and the in-situ observations, incl. WMO standards. They provide continuous total column observations, but have sparse coverage. The various observation techniques have been used in case studies [25, 27, 9, 13, 17, 14, 30, 31, 32] to estimate sources or sinks of the greenhouse gases CO_2, CH_4, and N_2O, but they have by far not been fully exploited in a combined manner. The missing element required for ITMS is the tailoring of the in-situ and remote sensing data sets to the ITMS needs, their consistent quality control, the continuous characterisation and mitigation of systematic errors in the satellite remote sensing data products at high spatial resolution, as well as research to improve observation capabilities at the sub-national scale according to ITMS needs.

An overall research challenge of ITMS is how the different observational data sets and capabilities can be combined to improve emissions estimates from point source scale to the national scale, ideally consistent with larger scale (European, global) approaches. Modules B meet this challenge from the observing system perspective, tailored to the needs of atmospheric inverse modelling (Module M) and exchange flux process understanding (Module Q&S). Special emphasis is on the usage of tracers (e.g. 14C, CO, NO_2) to separate emission processes and emissions from different sectors. One key issue to be addressed in Modules B is the error characterisation and data quality improvements on sub-national scale down to local scales.

An important overarching task within Module B will be the systematic assessment how the observation systems can be further optimised and developed in support of ITMS needs and requirements. This will include the identification of critical observational gaps and the assessement of new observational approaches.

The work of Module B (“Beobachtung”) is split into ***Module B_I: Core greenhouse gas observational data sets*** and ***Module B_II: Called greenhouse gas observational data sets.***

Module ITMS-B_I will develop and provide GHG in-situ concentration and total column data tailored to the needs of an integrated greenhouse gas monitoring system for Germany as well as land surface data for surface flux upscaling. The module relies on existing data sources (ICOS, IAGOS, TCCON, satellite data, etc.). It will prepare quality controlled in-situ and remote sensing data matched for optimally use with the inversion systems (with Module M) and/or to support flux model development and assessments (with Module Q&S).

Module B_II focuses on new observational approaches for future use within ITMS and/or in support ITMS data quality assessments (incl. emission quantification).

5.2.1 Module B_I

WP-B_I.1 Observation Data Synthesis and Coordination

<u>Responsible partner:</u> **UBre**, Dr. Heinrich Bovensmann, Dr. Michael Buchwitz

Main focus of this activity is to ensure that observational data from Module B are fit for purpose for the usage within ITMS in terms of interfaces and data quality. This will include the harmonisation of interfaces, the coordination of campaigns (called WPs within B_II) as well as the identification of observational gaps and initiation of steps towards closing critical observational gaps by improving the observation system in the future. This work package will also support Module K (overall ITMS Coordination), will organise regular meetings of Module B partners as well as perform the reporting including regular reporting on Module B milestones and deliverables in cooperation with the Module B work package leads. Main outputs are yearly Observation Data Synthesis Reports as well as inputs to IMTS reporting and benchmarking.

WP-B_I.2 Provision of In-situ Concentration Data from ICOS and IAGOS Tailored to ITMS Applications and Extension of ICOS Tall Tower Measurements

<u>Responsible partner:</u> **DWD**, Dr. Dagmar Kubistin, Dr. Jennifer Müller-Williams

This WP supports the provision and QA of in-situ concentration data from ICOS and IAGOS. This includes for IAGOS greenhouse gases (CO_2, CH_4, partly N_2O) as well as reactive gases (O_3, CO, NO_x, NO_y) along flight corridors. For ICOS it will include, beside the continuous monitoring of atmospheric greenhouse gas (GHG) concentrations (CO_2, CH_4, CO, N_2O, ^{14}C) at the atmospheric stations (mostly tall tower), the upgrade of selected atmospheric tall towers with NO_x measurement capabilities to provide an additional tracer sensitive to CO_2ff sources. ICOS data are provided for all 9 tall tower stations by DWD, 2 mountain stations and one marine site by UBA and IAGOS data for all IAGOS starts and landings at German airports with the GHG package on board. Main output are quality controlled ICOS and IAGOS data for ingestion into the ITMS system.

WP-B_I.3 Provision of Ground-based In-situ Data from ICOS and TERENO Ecosystem Sites

Responsible partner: **Thünen Institute**, Dr. Christian Brümmer, Dr. Frederik Schrader

This WP supports the provision of in-situ concentration and flux data from ecosystem sites from ICOS and TERENO stations for process characterisation and modelling within Module Q&S. This will include fluxes for CO_2, H_2O and CH_4, N_2O where available from eddy covariance measurements as well as related ecosystem parameters [15]. Ecosystem data (ICOS, TERENO) are provided for the existing stations and when available for new stations via the ICOS and TERENO data portals. Main output are quality controlled ICOS and TERENO ecosystem flux data as input to Module M and Module Q&S.

WP-B_I.4 XCH_4 S5P Satellite Data Tailored for ITMS Applications

Responsible partner: **UBre**, Dr. Michael Buchwitz, Dr. Oliver Schneising-Weigel

Atmospheric XCH_4 fields from satellite remote sensing are planned to be assimilated by ITMS. This WP focusses on the optimisation of S5P XCH_4 for applications at and below the national scale. It will provide quality controlled data with minimised systematic errors at high spatial resolution and dense coverage for Germany and surrounding areas. In this WP detailed comparisons of the latest S5P XCH4 data products will be carried out focussing on Germany and surrounding countries and it will be investigated to what extent the products can be further improved for ITMS applications. This includes optimized quality filtering and bias correction to enhance the yield (coverage) and to minimize biases. This also includes detailed uncertainty characterization and validation (TCCON, COCCON when available). In case issues are identified with the operational product, feedback will be given with the potential to improve also the quality of the operational product. As S5P data is available from early 2018 onwards, this WP will generate a 5-year data set optimized for central Europe. It will also be investigated to what extend changes in terms of atmospheric concentrations and / or emissions can be detected and quantified. If successful, this approach will then be used to verify changes in emissions determined by ITMS. Main output are quality controlled XCH_4 data tailored to ITMS needs for Module M and time series analysis of changes in CH_4 concentrations and emissions.

WP-B_I.5 XCO_2 Satellite Data Tailored for ITMS Applications

Responsible partner: **UBre**, Dr. Michael Buchwitz, Dr. Maximilian Reuter

Atmospheric XCO_2 fields from satellite remote sensing are planned to be assimilated by ITMS. Currently only OCO-3 on ISS (successful launch 5/2019) [33] delivers images of XCO_2 over selected regions (e.g., coal fired power plants, cities) for selected times. From 2025/26 onwards, the European COPERNICUS CO2M mission is planned to provide such data regularly and with much better coverage. The focus of this WP is to exploit existing space-based observations of XCO_2 images (from OCO-3) and to optimally prepare for CO2M, also providing XCO_2 images. This WP focus on the use and optimisation of OCO-3 XCO_2 for applications at and below the national scale. For this purpose, the UBre FOCAL algorithm will be used, which has initially been developed for OCO-2 but is currently also used for GOSAT and GOSAT-2. This provides the possibility to improve data product quality and the option to generate an ensemble of products, e.g., obtained by varying relevant retrieval algorithm parameters, which can be used to characterize uncertainties introduced by the retrieval technique. Within this WP it is planned to use of simulate CO2M data to generate appropriate simulated CO2M Level 2 test data sets as input for Module M in addition to OCO-3 XCO_2 images. Main output are quality controlled XCO_2 data from OCO-

3 **Snapshot Area Maps** for selected regions in Germany and surrounding countries as well as simulated CO2M data, both as input to Module M.

WP-B_I.6 Satellite Data on Fossil Fuel Tracer CO and NO_2 Tailored for ITMS Applications

Responsible partner: **UBre**, Dr. Andreas Richter, Dr. Oliver Schneising-Weigel

CO_2 emission from fossil fuel combustion are accompanied by emissions of CO and NO_x, the latter quickly converting to NO_2. The ratio of CO and NO_x to CO_2 depends on the fuel and the combustion efficiency and temperature. CO and NO_x (NO_2) can therefore be used as tracers to identify different combustion processes and to distinguish between different combustion sources. Data assimilation of these tracers has the potential to help separating biogenic fluxes from fossil fuel CO_2 emissions. If emission factors are sufficiently well known, then derived emissions of these tracers (as obtained via inverse modelling) can also be used to obtain information on CO_2 emissions. However, such applications require appropriate information on atmospheric CO and NO_2 concentrations. Neither the operational tropospheric NO_2 product nor the operational CO column product are optimised for ITMS applications. The focus of this WP is therefore to generate appropriate NO_2 and CO data products from S5P focussing on Germany and surrounding countries. This includes detailed error characterization, validation and comparisons with other existing satellite-derived NO_2 and CO including the operational S5P data products. To establish concentration ratios relative to CO2, model data (Modul M) or - where colocations are available - satellite-derived XCO_2 products (from WP-B_I.5) will be used. Concentration ratios will be analysed to answer the questions how far they can be linked to emission ratios. Main output are quality controlled XCO and tropospheric NO_2 data tailored to ITMS needs, computation and analysis of concentration ratios and comparisons with emission ratios.

WP-B_I.7 Land Surface Satellite Data Tailored for ITMS Applications

Responsible partner: **MPI-BGC**, Dr. Gregory Duveiller

Up-to-date spatially explicit CO_2 fluxes between the ecosystems and the atmosphere ("gridded fluxes") at high spatial (< 10 km, goal 1 km) and temporal (hourly) are an important basis of ITMS. They can be derived by a data-driven bottom-up approach. With machine learning, eddy covariance measurements, climate data and satellite data can be mapped onto spatially distributed CO_2 biosphere fluxes, an important input ITMS-M and to be generated in WP3 of the ITMS-Q&S_I Module. The present work package in Module ITMS-B_I is to establish a flexible and operationalizable workflow for acquiring and processing the relevant satellite based land surface data for the estimating high spatial resolution, hourly biogenic CO_2 fluxes through the integration of machine learning of satellite data and ecosystem measurements by ITMS-Q&S_I WP3. The request for funding here has a focus on the development of a semi-operational workflow for the acquisition and processing of satellite data, as this operational aspect is not funded otherwise. Main output are space-time fields of various surface satellite data for the regional domain as well as extracted time series for ecosystem stations which are representative for German climate and geo-ecological conditions as input to Module ITMS-Q&S_I.

WP-B_I.8 XCH_4 MERLIN Preparation for ITMS Applications

Responsible partner: **DLR-IPA**, Dr. Andreas Fix

With the upcoming CH_4 lidar satellite mission MERLIN (launch planned 2027), XCH_4 data will become available with smaller systematic errors as from passive remote sensing system like S5P. The very small footprint (~100 m) reduces sensitivity to cloud cover, and the day and night measurement capability are further key assets for providing complementary data to S5P and S5 XCH_4. In the long term, both types of XCH_4 data are planned to be assimilated into the ITMS. Consequently, this WP focuses on the preparation of MERLIN XCH_4 retrieval for applications at and below national scale. It will provide synthetic XCH_4 MERLIN data and its error characterisation. It will also provide data to investigate the potential of deriving two pieces of information (above and below boundary layer columns using the Earth surface and cloud tops as the reflecting targets) on XCH_4 in the lower troposphere. Due to the nature of the IPDA lidar technique, the random error of a single measurement can be reduced or increased by appropriate averaging at the expense of spatial resolution. The optimum balance between resolution and error for best results within Module M will be subject to detailed analysis. Main output are quality controlled synthetic MERLIN XCH_4 data tailored to ITMS needs as input to Module M in preparation of Phase 2 data use.

5.2.2 Module B_II

i. **Provision and processing of ground-based FTIR spectrometer data for validation of satellite products and characterization of regional distributions and hotspot emissions**: On the one hand, column measurements from ground-based FTIR systems shall be provided and applied for validation, retrieval optimization, and error determination of satellite data from XCH4, XCO2, and XCO. Existing measurement networks (e.g. TCCON) in Germany shall be complemented by regional measurement networks and campaigns of mobile FTIR in the area of important metropolitan areas (e.g. RheinMain, Munich) and important rural regions (e.g. Northwest Germany). Furthermore, regional gradients in atmospheric parameters shall be systematically recorded within campaigns for a reference year 2024 (TBC) coordinated within ITMS.

ii. **Improvement of emission estimates for methane for specific source types (measurement campaigns):** Determination of methane emissions from unknown, localized sources (e.g. landfills, biogas plants, gas production, etc.) using existing measurement infrastructure (e.g. mobile in-situ and remote sensing sensors each from ground or air) as well as simple modelling approaches (e.g. mass balance methods) and comparison with bottom-up estimates for the respective source. Derive emission guidance values for specific source types. Source types shall be selected in consultation with the ITMS consortium and the Federal Environmental Agency.

iii. **Improvement of emission determinations for CO2 on local, urban and regional scales, especially in metropolitan areas (measurement campaigns):** determination of atmospheric concentrations of CO2 and relevant tracers using existing measurement infrastructure (mobile in-situ and remote sensing sensors each from ground or air) and simple modelling approaches (e.g. mass balance methods). Comparison with bottom-up estimates and derivation of emission benchmarks. The selection of the agglomerations (measurement campaigns) shall be done in consultation with the ITMS consortium and the German Federal Environmental Agency.

iv. **Characterization of the spatial GHG concentration variability of a region in Northwest Germany (measurement campaigns):** In addition to existing measurement stations (ICOS station Steinkimmen and TCCON station Bremen) in Northwest Germany, systematic measurement flights shall be performed to record atmospheric concentrations of CO2, CH4, CO, and N2O in the region of Northwest Germany with its extensive agricultural areas, the urban centers Bremen and Oldenburg embedded in it, and the gas and oil production present in the area, whereby the entire boundary layer shall be probed. The data should make it possible to record the emissions of important sectors (see above), in particular also for N2O.

v. **Feasibility study of the Virtual Tall Tower concept using ecosystem monitoring sites:** the activity should answer the question of whether ecosystem station data and local modeling (to be developed in study) can be used to estimate GHG concentrations in the boundary layer with comparable quality to those at tall towers, making more "base points" available for inverse modelling. The investigations shall initially be carried out for CO2 as an example. The quality of this approach is to be documented by comparisons with, for example, neighbouring ICOS atmosphere stations. If the demonstration is successful, the feasibility for other GHGs is to be assessed and the transferability to the entire German ecosystem measurement network is to be investigated.

vi. **Isotope-specific quantification of GHG and water vapour:** Significant uncertainties remain regarding the spatio-temporal variability of evapotranspiration, CO2, CH4 and N2O fluxes between terrestrial ecosystems and the atmosphere. Observational data from isotope-specific sensors offers the opportunity to reduce these uncertainties since isotope analysis decomposes the total flows into their components. Therefore a feasibility study to characterization of the influence of spatio-temporal variability of evapotranspiration on CO2, CH4 and N2O fluxes between terrestrial ecosystems and the atmosphere shall be established. The feasibility shall be demonstrated for at least one representative

ICOS ecosystem station and the usefulness of the method for ITMS and extension to other ecosystem stations shall be discussed and evaluated.

5.3 Modules Q&S: Sources and Sinks of GHG

The overall objective of the ITMS module Q&S is to provide "bottom-up" inventories of sources and sinks of GHGs (here: CO_2, CH_4, and N_2O) associated with fossil energy use and waste treatment (e.g., energy sector, industry, transport, household, and waste management) as well as land use, agriculture, and forestry. To this end, the basic processes for the source and sink behavior of the various GHGs in the aforementioned sectors need to be better understood and characterized. Innovative methods for an improved spatio-temporal characterization of these sources and sinks via "bottom-up" approaches will be developed.

In the first phase of ITMS, the work of Module Q&S ("Quellen&Senken") is split into ***Module_Q&S_I: Core sources and sinks of greenhouse gases*** and ***Module_Q&S_II: Called sources and sinks of greenhouse gases.*** Given the importance, huge diversity and non-point characteristic of biogenic GHG sources (and sinks), the provision of a-priori emission fields at national scale does not only require an improved characterization of energy production, transport, household and industry related sources, but also a detailed quantification of GHG fluxes related to agricultural and forestry activities, land use and management changes (e.g. restoration or re-wetting of organic soils) and GHG exchange between surface (incl. coastal waters) and the atmosphere. The non-energy related GHG fluxes are mainly due to biogenic processes, which are due to its dependence on environmental factors such climate, soils, plant performance or microbial communities etc., characterized by a high spatial and temporal variability. Describing the dynamics of the biosphere-atmosphere exchange of biogenic GHG sources and sinks in high spatio-temporal resolution will thus require advanced, innovative modeling approaches, which are capable to simulate the biogenic processes associated with the production and consumption of atmospheric CO_2, CH_4 and N_2O. Therefore, the main focus of Module Q&S is given to the testing, further development and comparison of existing empirical, semi-empirical and process-oriented modelling approaches, capable to describe the biosphere-atmosphere exchange processes of GHGs across managed landscapes and regions (incl. coastal environments). This also includes a thorough assessment and communication of uncertainties of spatial and temporal predictions used as a-priori for ITMS. In addition, current GHG inventory data used for UNFCCC reporting should be further refined regarding its spatio-temporal resolution and made available for comparison with other bottom-up and top-down approaches for GHG inventorying within ITMS.

5.3.1 Module Q&S_I

WP-Q&S_I.1 GHG emissions by the sectors industry, transport, energy and waste

<u>Responsible partner:</u> **UBA**, Dr. Dirk Günther / Dr. Christian Mielke

In this WP the Umweltbundesamt will work on spatio-temporal downscaling of anthropogenic emissions from the sectors industry, transport, energy and waste.

<u>Tasks:</u> Identifying the essential parameters (activity data and emission factors) driving spatio-temporal patterns. Assessment of uncertainties (incl. assessment of co-variations). Development of emission maps for the years 2005 to 2020, which however will still be coarse (e.g. monthly at best) and not fully comply with spatio-temporal demands of the ITMS system. Comparison and harmonization of spatiotemporal scaled emission fields with other data sources (TNO Bottom-up emission estimates for anthropogenic CO_2 and with other data sources (e.g. TNO co-emitted tracers at 5 km)). Development of temporal activity fields for various source categories. Operationalization and integration of data in ITMS system.

WP-Q&S_I.2 GHG fluxes for agricultural and forest sectors

<u>Responsible partner:</u> **Thünen (TI)**, Dr. Christian Brümmer

In this WP Thünen Institute delivers spatial downscaled GHG National Inventory Reporting data (NIR) for the sectors agriculture, forestry and land use (AFOLU).

The project will deliver spatial downscaled CO_2, CH_4 and N_2O emission fields based on national UNFCCC reporting according to the "Nationalen Inventarbericht", thereby differentiating between the various source categories such as livestock systems, direct soil emissions, indirect emissions and emissions due to landuse change.

Input data will be taken from National Inventory Reporting (NIR) on GHG emissions from AFOLU (GasEM), statistics on fertilizer use and agricultural management, national forest inventory data, livestock systems information incl. manure management schemes. The major output will be a dynamic database system on AFOLU GHG emissions for ITMS, thereby as well providing coarse information on agricultural and forest management. How much details will be provided, will as well depend on the results of an evaluation of existing data protection guidelines.

WP-Q&S_I.3 Biogenic CO_2 fluxes

<u>Responsible partner:</u> **MPI-BGC**, Dr. Gregory Duveiller

This work-package will set-up a flexible and operational workflow to estimate hourly biogenic CO_2 fluxes at high spatio-temporal resolution on basis of the integration of machine learning, satellite data and measurements of CO_2 fluxes and supplementary parameters at eddy co-variance sites in Germany. This will serve as a prior for the inversion activities of the ITMS-M module. This work leverages on the long expertise of the MPI-BGC group related to the FLUXCOM initiative (www.fluxcom.org).

Main tasks are associated with the consolidation of all necessary input information for training the machine learning methodology into a structured database. Aggregation of information and development of a suitable data structure allowing for machine learning. Production of emission fields of biogenic CO_2 fluxes based on the calibrated algorithms.

The WP requires as inputs datasets of land surface satellite products specifically tailored for ITMS (ITMS-B_I.WP7). Moreover, meteorological gridded data and eddy covariance site data and ancillary information from ITMS-Q&S_I.WP2 will be needed. WP-Q&S_I.3 is provisioning a structured database for machine learning and a first version of algorithms tested for limited dataset. It will deliver first data of estimated land biogenic CO_2 fluxes.

WP-Q&S_I.4 Biogeochemical modeling of ecosystem GHG exchange

<u>Responsible partner:</u> **KIT-IMK-IFU**, Prof. Dr. Klaus Butterbach-Bahl

This WP will provide high spatio-temporal emission/deposition fields for CO_2, N_2O, and CH_4 for agricultural and forestry landuses and natural land (wetlands) of Germany. The WP will use advanced biogeochemical models linked to spatial explicit information on landuse, land-management, soil properties, vegetation characteristics and meteorological conditions to calculate in spatio-temporal emission/deposition fields for CO_2, N_2O, and CH_4 for all major terrestrial ecosystem types (forest, arable land, grassland, wetlands). Relevant input and activity databases will be developed in cooperation with WP_Q&S_1.2 and 1.3, with information being synthesized and made available for modelling at regional and national scale. Test dataset from ICOS, TERENO and other sites will be used for model testing and for assessing structural and parametric model uncertainties. Based on simplified assumptions on activity data (land and forest management) first GHG inventories will be calculated and a suitable input-output data structure for ITMS will be developed.

Required input relates to harmonized data from the GHG observational network ICOS/TERENO and other long-term observational sites (ITMS-B workpackages); advanced datasets on processes and GHG fluxes as supposed to be delivered by ITMS-Q&S_II and activity data by e.g. ITMS-Q&S_I.2 and ITMS-Q&S_II. The WP will deliver tested biogeochemical models with assessed and documented structural and parametric uncertainty as well as first coarse a-priori emission fields on terrestrial ecosystem CO_2, N_2O, and CH_4 fluxes.

5.3.2 Module Q&S_II

The research fields and work packages outlined are based on research gaps identified by the research community and by the ITMS consortium. These gaps in information needs to be addressed to finally be able to deliver on the overall objectives of ITMS and specifically of those of Module Q&S. The following work packages are expected:

i. High-resolution spatio-temporal CO_2 and CH_4 emission maps for the sectors industry, transport and waste management. Establishment of an operational, real-time system of high-resolution (first phase: 7 km x 7 km, hourly) emission maps for greenhouse gas emissions from the mentioned sectors, in cooperation with relevant UBA activities.

ii. High-resolution activity data for the sectors agriculture, forestry, and land use (AFOLU): improved spatial (<1 km^2) and temporal (10-20 days) information on land management as basis for empirical or process-oriented approaches to estimate GHG fluxes from agricultural and forestry land uses. Various observational (e.g. remote sensing), statistical data or other sources (e.g. surveys) may be used to describe land management. Existing information on land-use and management may be restricted due to data-protection policies, so that it may be necessary to settle agreements with state authorities for using high resolution spatial data on land management. Therefore, in the first phase, this barrier should be addressed and resolved for at least two federal states.

iii. GHG emissions from livestock systems in Germany. ITMS requires improved spatio-temporal estimation of GHG emissions from livestock production systems. For this, existing approaches such as the GasEM model, which is used for the national UNFCCC reporting according to the "Nationalen Inventarbericht" may be refined. Existing barriers on data use may restrict the development of a national approach in the first phase of ITMS. However, data use restrictions should be resolved for at least two federal states, and detailed information on animal numbers, livestock production systems and manure management in high spatio-temporal resolution (first phase: 7 km x 7km, monthly to seasonal) shall be provided.

iv. Estimation of biogenic CO_2 emissions: Based on existing data (in-situ and remote sensing sources), tests and uncertainty analyses of artificial intelligence (AI) systems shall be developed, which allow the characterization of the relationships of the different data of CO_2 fluxes. It is expected that this will lead to an improved estimation of biogenic CO_2 emissions for Germany (and adjacent areas) and enable the operationalization of such a system for integration into the ITMS system.

v. Biogeochemical modeling of GHG exchange processes: Use of biogeochemical models to simulate biosphere-atmosphere exchange of GHGs (CO_2, CH_4, N_2O) between agricultural and forest ecosystems and the atmosphere to generate high temporal resolution GHG flux fields (up to 1 km^2, hourly) for entire Germany and neighboring regions. The modeling approach needs to include regional uncertainty analyses and be operationalized for integration into the ITMS system.

vi. Modeling of GHG emissions from peatlands and organic soils: Using process-based modeling approaches, GHG emissions from natural, drained and rewetted wetlands should be estimated for Germany at high spatio-temporal resolution (at least 7 km x 7 km, hourly). Land use activities, leaf area index developments, groundwater, and other environmental parameters may be included to assess GHG exchange between wetlands and the atmosphere.

vii. Analysis of GHG emissions from coastal regions and surface waters: Development of approaches for generating high spatio-temporal resolution GHG flux fields (minimum 7 km x 7 km, hourly) for German coastal areas (and possibly inland waters) on basis of measurements and modeling.

viii. Soil carbon storage: analysis of existing approaches, synthesis and further development of innovative parameterization and measurement approaches to capture and simulate ecosystem-level greenhouse gas exchange, and development and testing of approaches to improve estimation of temporal changes in soil carbon storage of agricultural ecosystems.

ix. ^{222}Radon emissions from soils: development and testing of modeling approaches at site scale for estimating ^{222}Rn emissions from soils. Development of temporal-spatial (0.01° resolution, 1h) high-resolution emission inventories for the ITMS domain.

x. Biogenic sources of CH_4: Develop and test measurement and modeling approaches to identify and disentangle various biogenic sources of CH_4 (ruminant emissions, farm manure storage, wetlands) at farm to regional scales based on isotopic signatures.

5.4 Module K: Coordination

Module ITMS-K (i.e., COORDINATION) coordinates the overall ITMS, focusing on reaching the demanding objectives of ITMS by coordinating and controlling activities within each module and fostering an optimal interplay between all ITMS modules.

All project participants and their work in the different modules are to be effectively coordinated with the goal to achieve the defined overall project Milestones. Communication, meetings and controlling are organized in a way that the Deliverables and Milestones are met in time, critical contributions and bottlenecks are identified and the associated risks mitigated.

In practice, the tasks of ITMS-K are organised in five Work packages:

WP-K.1 Communication and Meeting planning

WP-K.2 Project Reporting

WP-K.3 Benchmarking and planning for Phase 2

WP-K.4 Modules B observation data provision for use by other Modules

WP-K.5 Modules Q&S bottom-up flux data provision for use by other Modules

Efficient collaboration is fostered (WP-K.1). A Traceability Matrix is developed, success and bottlenecks are monitored and reported (WP-K.2). Progress is evaluated in WP-K.3 by means of benchmarking according to the project Milestones and Traceability Matrix. WP-K.4 is concerned specifically with Modules B linkages within the overall project, and WP-K.5 with Modules Q&S linkages within the overall project.

The challenges of ITMS-K are that several different research communities have to bundle their efforts. The linear developments in WPs and Modules need to be connected to other activities in a complex matrix of inter-dependencies. The system has to remain flexible with respect to developments of state of science, available tools, yet to be investigated potentials and limitations of data and models, and to respond to possible changes in user requirements.

5.5 Module V: Utilization and Communication

Module V will provide custom-tailored communication of results for a variety of users and stakeholders (from politics, government agencies and public), this includes visualization of results with web-based applications as well as communication of results in connection with the national GHG reporting (NIR), all to be embedded in a long-term stewardship. The aims are in particular:

1. Satisfy the needs of the users, in particular of the core users, which are agencies concerned with GHG emissions
2. Communicate user requirements to the Modules M, B, Q&S, with special emphasis on coverage and spatial as well as time resolution
3. Establish online result dissemination for the benefit of a variety of users

4. External communication is foreseen with core users, stake holders, and with potential users at meetings, as well as targeted personal communications. Communication with the public will use traditional publications like press releases and social media to the extent to which they may be applicable.

GHG information needs to be provided in clear, comprehensible products representing appropriately the science behind ITMS and at the same time in an easily understandable way for all kinds of users.

5.6 Expected results of Demonstration Phase

5.6.1 Exploitation of ITMS results for governmental agencies

The ITMS project is creating a data and knowledge transfer between the scientific community and governmental agencies , aiming for an operational system which will be of multiple uses for the governmental agencies DWD, UBA, and Thünen-Institute. All three agencies have been involved in the planning of the ITMS project from the very beginning, and are willing to provide in-kind contributions of both data and manpower to ensure the success of ITMS.

For several years, DWD (Deutscher Wetterdienst, of German weather service, subordinate to BMVI) is strongly involved within ICOS, responsible for the implementation and operation of the atmospheric network, therefore securing a fundamental data stream for ITMS as an in-kind contribution to Module B. Concerning the modelling (Module M), the ITMS will allow for the first time to use the new operational numerical weather forecasting model of DWD (ICON) as a superior transport model for inversion purposes. Results of the ITMS are planned to be exploited within the DWD's operational emission verification. For the dissemination of ITMS results, DWD offers synergies with its standard weather and climate data service.

UBA (Umweltbundesamt, or Federal German Environment Agency, subordinate to BMU, the Federal Ministry for the Environment, Nature Conservation and Nuclear Safety), is responsible for the UNFCCC inventory reporting for Germany. These national inventories have been under responsibility of UBA for almost 20 years, resulting in both high expertise, proprietary information and an enormous and steadily growing collection of information on emissions and activity data for Germany since 1990. By means of the ITMS project, this data collection will in substantial parts be made available to the scientific community. On the other hand, UBA is interested to benefit from ITMS research, especially for diffuse fugitive and land-based emission sources. UBA is a partner within the VERIFY H2020 project since 2018, thus can draw on the experience at the European scale as well. UBA 's involvement in Module Q&S research is connected with the in-house Gridding Emission Tool ArcGIS (Greta) for creating spatio-temporally resolved GHG emission maps consistent with the NIR emission inventories, for use within the ITMS. Concerning exploitation of ITMS results, it is foreseen that UBA regularly adds ITMS results as emission verification to their National Emission Report (NIR), similarly as already practised in the UK and Switzerland. UBA also intends to use ITMS results for improving emission inventories on source base.

The Institute of Climate-Smart Agriculture within the Thünen Institute, subordinate to BMEL (Federal Ministry of Food and Agriculture), is tasked by UBA (BMEL) for the annual reporting calculation of emissions from agriculture, land use and land-use changes (LULUCF) in the context of the National System on Emissions, coordinated by UBA. Using the GAS-EM inventory model, they also quantify performance-based mapping of emissions from animal husbandry. There is strong interest in contributing to ITMS research, specifically within Module Q&S, and in making use of the observation derived GHG emissions provided by the ITMS.

Close involvement during the ITMS Demonstration Phase lays the foundation for optimal exploitation of ITMS results within the operational services of DWD, UBA, and Thünen-Institute.

5.6.2 Synergies with other projects

This ITMS work plan ensures that synergies with other research activities are identified and utilized. In the following section, various relevant research projects and their synergies with the ITMS research activities are listed.

As already pointed out in previous sections, a number of projects are active in the area of GHG monitoring at the European level: ICOS, IAGOS, Copernicus (CAMS, C3S, CO2M), MERLIN, and the H2020 projects CHE, VERIFY, CoCO2, and the upcoming project PAUL. Especially within CHE and VERIFY first steps are taken towards an operational observation-based system for monitoring and verification of greenhouse gases, targeting the European scale, with the aim to implement an operational system in the European Copernicus Services. The results and experiences from these three projects will be used for the national ITMS research project through the participation of several ITMS partners in CHE, VERIFY and CoCO2, but cannot be directly transferred due to the different methodological approaches and different scales. Discussion with CAMS representatives have already started to ensure an appropriate cooperation between CAMS and ITMS, with the overall agreement that support for GHG reporting at national scale and below is regarded as a “downstream service” to CAMS, and should be provided through national GHG monitoring systems such as ITMS. From 2021-2023 the H2020 project *Prototype system for a Copernicus* CO_2 *Service* (CoCO2) is running with involvement of several ITMS partners, comparing methods on the European and national scale, allowing synergies w.r.t. CO_2 emission estimation. Close collaboration with respect to method development is desirable, especially concerning GHG data assimilation. Links will be fostered, e.g., by appointing ITMS Scientific Advisory Board members from the respective EU projects’ steering group members. Within the upcoming project PAUL (Pilot Application in Urban Landscapes), a project proposed within the H2020 Green Deal Call, capabilities for observing and quantifying GHG budgets on the city scale will be developed. Clear synergies with the assessment of urban scale observing systems for anthropogenic emissions within Modul M will be utilized. Furthermore, pilot implementations within PAUL for the city of Munich, if successful, will be relevant for developments of the ITMS within future phases.

Also related, the National Copernicus Project „Hochaufgelöste anthropogene Treibhausgasemissionen aus Copernicus-Diensten für Bundesländer, Landkreise und Städte Deutschlands“ (HoTC) running 2021-2023, is preparing the inclusion of Copernicus data into both modelling systems and data service systems of DWD. The resulting synergies will be utilized in Modules M and Q&S.

The collaborative project providing NDACC and TCCON data for the validation of Sentinel 5-precursor (funding code 50EE1711, until Sept. 2021) has obvious potential for synergy. Parts of the validation data needed within ITMS WP1.3 will come out of this collaborative project in the early part of ITMS Phase 1.

During the first ITMS research phase, strong collaboration will be established with the DFG-funded project “Mesoscale network for monitoring greenhouse gas and pollutant emissions“ (Project number 419317138), which will set up an atmospheric column measurement network using mobile FTIR spectrometer around Munich as part of COCCON. The research proposed within WP1.5 and WP1.9 will certainly benefit from a close collaboration with the research group involved with this mesoscale network.

Also during the first ITMS research phase, the strong collaboration with ESA on S5P and CO2M product development will be continued, with the goal to ingest algorithm improvements demonstrated to be important for and needed by ITMS into the operational processing chains. Existing involvement in the S5P Quality Working Group, the S5P Mission Performance Centre and the CO2M Mission Advisory Group (and related project) are enabling direct contact with ESA and EUMETSAT to stimulate uptake of ITMS results on algorithm improvements. It is expected that ITMS will trigger further European instruments for active (lidar) monitoring of CO_2 and CH_4 from space as a complementary measurement principle wrt. passive spectrometers with large potential for synergistic retrievals to advance a better understanding of the natural carbon cycle and its disturbances by anthropogenic emissions.

Methods and sensors developed and currently under development within the AIRSPACE project (FKZ 01LK1701) will be used within ITMS.

Some institutions of the ITMS community are also involved in the BMBF-funded „Verbundprojekt Stadtklima" where synergies can be expected with respect to observations and modelling of atmospheric processes in cities. Together with the results of the BMWi project iZEUS (intelligent Zero Emission Urban System), ITMS could observe, model and visualize the success of emission mitigation of individual cities. The results of the current BMBF research project CLIMEXTREME could be used within ITMS to estimate expected changes in sources and sinks through climate change, this way establishing an early warning capacity. First inventories of GHG fluxes between terrestrial ecosystems (agriculture and forestry) with Landscape DNDC for Saxony and entire Germany were calculated e.g. in the frame of the EU project NitroEurope, so that preliminary spatial data on land use and land management are available.

The ITMS is designed to be compatible with the Earth system modelling strategy currently discussed in Germany at the level of institution heads under the umbrella of Deutsches Klimakonsortium (DKK). ITMS will contribute with developments w.r.t. passive tracer transport, paving the way for future atmospheric chemistry modelling.

The ITMS, especially its atmospheric and isotopic monitoring components, will be complementary in its longer-term nature to the efforts undertaken in the Helmholtz-funded observing systems TERENO and MOSES, with foci on assessing long-term changes in ecosystem functioning and fluxes as affected by climate change and on short-term effects of extreme events (drought, flooding) on terrestrial, aquatic and marine ecosystems and their exchange fluxes with the atmosphere.

5.6.3 Expected achievements of Phase 1 (Demonstration Phase)

With the ITMS as a funded project, a consolidation of national research activities can be anticipated, a closer collaboration of observing and modelling communities and research efforts focused on exploitable results. Scientific progress can be expected with observation strategies, observation exploitation, especially better information use of satellite data, increased capabilities in modelling and inversion techniques, as well as enhanced understanding of sources and sinks of GHGs, particularly in the agricultural sector (both animal husbandry and crops).

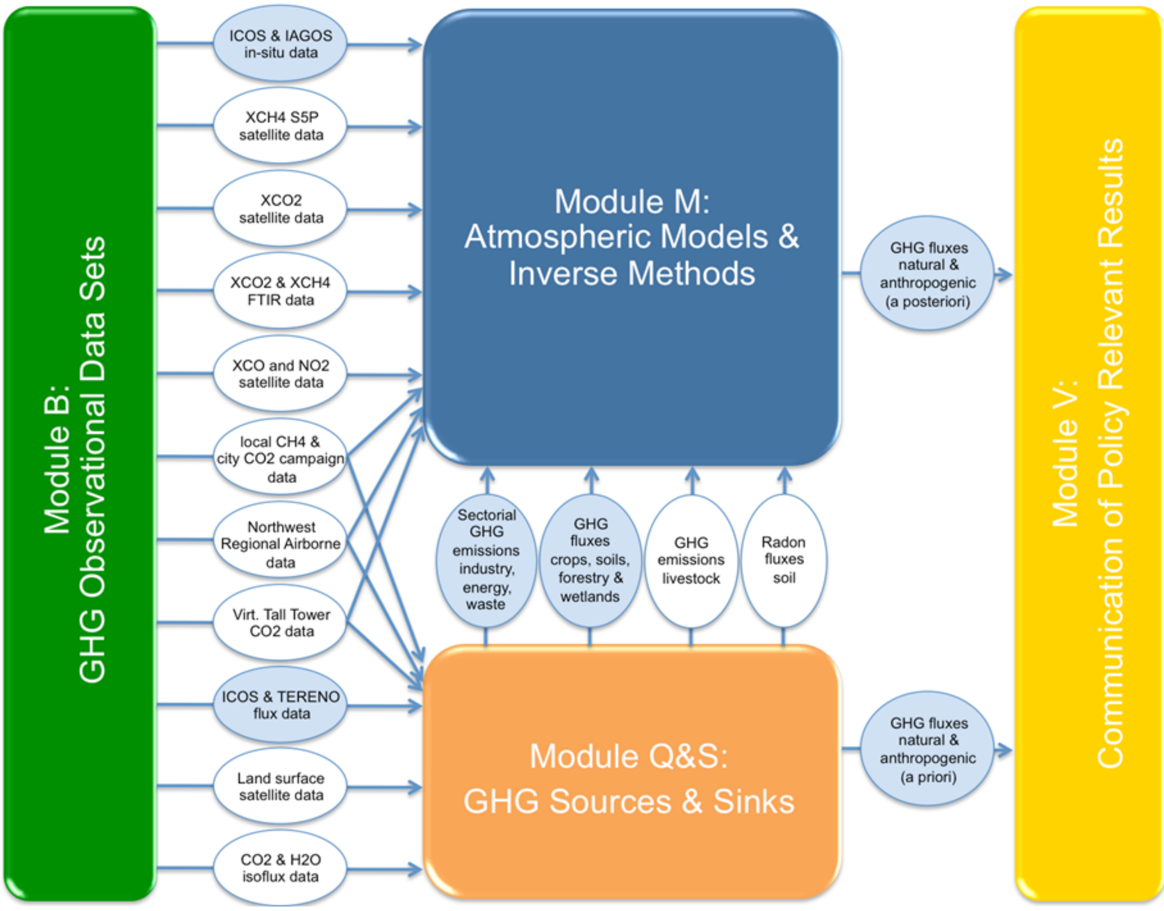

Figure 7: Simplified data flow between the Modules, with early implementation (i.e., at first milestone MS-ITMS.1) shaded in blue. Note the overall Coordination (Module K) is not shown.

ITMS will provide emission estimates in accordance with observations. It will provide results, on the one hand, combining observations with reported inventories for best estimates, and it can, on the other hand, provide independent estimates for verification purposes. ITMS will link observed concentrations to emission fields, separating the GHG fluxes from sources within Germany from GHG fluxes advected by transport from outside the domain. ITMS allows visualization and monitoring of hot spots, giving support to political decision makers and informing the public. ITMS will be crucial for monitoring, reporting and verification (MRV) for GHG emission reductions needed for the agricultural sector and, thus, also for determining tangible reduction goals for NDCs. A respective tool will be provided for governmental institutions and NGOs.

Specifically, after Phase 1, a pre-operational "Demonstrator" ITMS will be in place providing information on GHG sources and sinks to users, agencies, and the public on a regular (annual) basis. These pre-operational products will be generated through the regular exchange of data between Modules B, Q&S, and M. The stepwise enhancements in observational data streams within Modules B, in a-priori flux estimates in Modules Q&S, and in the data assimilation in Module M will result in increasing robustness of the products throughout the ITMS development.

5.6.4 Measures of success for ITMS Demonstration Phase

The five overarching Milestones ITMS1-5 (see Fig. 5) serve as top-level indicators for the success of the developments during the Demonstration Phase of ITMS. The individual Module-related Milestones and the Workpackage - specific Deliverables feed into the overarching Milestones. Thus, the success of each task and its contribution to project success is traceable. It is the task of Module K to track the progress.

During the course of the project, a Traceability Matrix will be established as part of the tasks of Module K. This is meant as a high-level document, that will on one hand trace the user requirements according to use cases. On the other hand, the Traceability Matrix traces the capabilities of the ITMS system. Relating both allows evaluating the adequacy of observations, data bases and respective modelling capabilities and identifying areas of improvement. The Traceability Matrix measures the usefulness of ITMS for selected applications. The Traceability Matrix will be a living document and shall be adapted to changing requirements and capabilities over time. It will be a tool for measuring the success of ITMS also in subsequent ITMS Phases, growing with the number of applications.

6. Project Phase 2 (First Generation ITMS)

6.1 Envisaged research in subsequent Phase 2

To develop the ITMS from the demonstrator stage (at the end of Phase 1) to a potentially operational system (First generation ITMS), a strong effort is needed in all Modules during Phase 2, for pushing to increased quality and resolution, thus enabling new products, and perpetuate those for new users. As Phase 2 will comfortably benefit from the scientific achievements of Phase 1, the logical Module structure will remain the same. It can be expected that in the meantime the progress in the Copernicus Services allows to reduce the domain size and increase spatial resolution at the same time, without significantly increasing computational costs. It is anticipated that every increase in resolution (spatial, sectorial, or w.r.t. uncertainty) enhances user uptake. However, it is foreseen that in addition to scientific and data output, a number of products could be derived, such that user do not need scientific background for ITMS result application.

The ultimate aim is to have an operational ITMS providing regular information on GHG sources and sinks. It is envisioned to establish the long-term operation of the ITMS at public agencies such as DWD, UBA, the Thünen Institut, and possibly CMSAF (EUMETSATS Climate Monitoring Satellite Application Facility). The current aspiration of DWD to move ICON towards an Earth System Model would make Phase 2 developments a perfect timing with a good chance of feeding into the subsequent ICON model family with permanent usage. At the same time, ITMS is envisioned as a platform for researchers to apply ITMS developments to upcoming scientific questions. For example, a version of the operational data GHG assimilation system could be used in combination with additional local observations to investigate regional/local scale emissions, or with new types of observations (e.g. drone data, or new satellite concepts) to assess their potential information content on GHG fluxes.

To achieve this, development will be needed in all ITMS Modules. Below are some examples of potential Phase 2 developments. Details will be discussed in context of the Milestone "Status review and planning of Phase 2" foreseen for month 38 of Phase 1.

The ICON GHG data assimilation at DWD needs to be fully developed from a demonstrator to a first-generation operational system, such that regular reporting of top-down constraints can be taken over from the CSR system early in Phase 2. The pre-operational CSR system will be continued as a reference system to ensure consistency in reporting GHG flux estimates across the multiple development steps. Potential developments in Phase 2 are the implementation of a process-based biosphere model within ICON (benefitting from the CSR system), the development a Carbon Cycle Data Assimilation System (CCDAS), incorporating of land use data, also exploring the potential of an FFDAS (fossil fuel data assimilation), the feasibility of which has been demonstrated before with other models, e.g. [34],[35]. New data streams need to be implemented for assimilation (e.g., also ground based column observations, N2O observations), the development of CCDAS), targeting top-down constrained flux controlling parameters within a flux model instead of simple corrections of prior fluxes, as well as FFDAS, targeting parameters controlling the emissions in an emission model, greatly enhance the usefulness of the data assimilation for providing information. Also the data assimilation needs to be further developed for urban areas, following up on the OSSE for urban GHG observing system in Phase 1 and on results from the PAUL H2020 project.

The provision of established and proven data streams from Phase 1 needs to be continued, but – building on lessons learned from Phase 1 and on new available observational data with high spatial and temporal resolution – the preparation and test usage of data from new sources will be valuable. This shall especially include the provision and assessment of new satellite data products and streams from Sentinel-5 (launch 2023), CO2M (launch 2026) and MERLIN (launch 2027) tailored to ITMS needs. In addition, the data provision of ICOS/IAGOS atmosphere data, ICOS/TERENO flux data, atmospheric and land surface satellite data as well as COCCON/TCCON need to be continued. New data products from S5 (XCH4, XCO2 (proxy), XCO, trop NO2), CO2M (XCO2, XCH4 images at 2 km x 2 km) and MERLIN (XCH4) need to be assessed and provided incl. adaptation of products and streams where necessary for ITMS purposes. Other potential developments include a feasibility assessment to use solar induced fluorescence from satellite data (S5, CO2M, FLEX) to constrain the biospheric part of the CO2 budget, and mobile ground and airborne observations focussing on - in Phase 1 underexplored - new source gases like N_2O and specific important source regions like urban areas.

Furthermore, in Phase 2 further improvement of the spatio-temporal resolution of GHG emissions related to the use of fossil fuels by integrating new information and advanced modelling approaches is envisioned. Phase I focused on the development and testing of approaches to obtain better spatio-temporal information on agricultural activities such as crop rotations, fertilization or livestock numbers on basis of assessing additional databases or by developing routines and extracting information from remotely sensed data (e.g. using SENTINEL I/II observations) for two federal states. Assuming that data privacy issues have been resolved and suitable satellite products and data processing chains have been developed, this approach will be expanded in Phase II to the entire ITMS simulation domain. It is expected that this will result in a further significant improvement of bottom up GHG flux fields for the agricultural as well as the forestry sectors. Phase II will also see the implementation of improved model versions for biogenic GHG emissions, e.g. with regard to narrowed uncertainties or improvements of the performance of the model within the ITMS systems. Embedding information on GHG emissions from the Fossil Fuel Data Assimilation System (FFDAS) and the Carbon Cycle Data Assimilation System (CCDAS) and the development of approaches to harmonize and supplement this information with results on CO_2 flux fields as obtained by ITMS are also potential topics of a Phase 2. Given the high sensitivity of biogenic GHG fluxes to changes in land management and climate, retrospective and prognostic model simulations at regional to national scales will be needed to better understand the function of soils and forest ecosystems as decadal sinks or sources for CO2. Also the potential of the ITMS system to monitor mitigation efforts of the agricultural sector to reduce GHG emissions and develop products to assess the effect of extreme events (e.g. droughts, floods) or regional forest damage on the regional and national GHG balance will need exploration.

Regarding the communication of results to users and stakeholders, a thorough user requirement analysis and use case collection will be developed, covering different technical background level of users as well as varying interest in scales and sectors. We aspire the involvement of research, commercial and public partners. Communication with partners and users with very different backgrounds (within the project and external) will require a setup of skilful information exchange, understanding the needs and restraints partners and users are placed in. Social science involvement is foreseen to enhance effective communication with commercial and public users on one hand, and on the other hand to understand and push the legal framework to make more data freely available, for the benefit of ITMS data usage as well as for open public data.

Product development will need to match the collected user requirements and the use case collection. Special focus will be given to shared language and easily understandable definition of products. Product development shall take place in close interaction with users. Each use case should be provided with at least one suitable product. Product development will make use or results of Modules M, B, Q&S, and should be suitable for operational continuation.

Benefitting from the lessons learnt from Phase 1, the project will continue to monitor the measures of success by means of the Traceability Matrix as defined and updated in Phase 1, and will add measures of success based on user requirement matching and user satisfaction. The new challenge is to build up management structures as well as internal and external data flow and communication structures which could run permanently, also after the Phase 2 has finished.

7. References

[1] Pinty B et al. 2017, An Operational Anthropogenic CO2 Emissions Monitoring & Verification Support capacity – Baseline Requirements, Model Components and Functional Architecture, doi: 10.2760/39384, European Commission JRC, EUR 28736 EN, http://copernicus.eu/sites/default/files/documents/News/Report_Copernicus_CO2_Monitoring_TaskForce_21122017.pdf

[2] 2019 Refinement to the 2006 IPCC Guidelines for National Greenhouse Gas Inventories, https://www.ipcc-nggip.iges.or.jp/public/2019rf/index.html , UNFCC 2019.

[3] https://www.gesetze-im-internet.de/ksg/BJNR251310019.html

[4] https://www.bundesverfassungsgericht.de/SharedDocs/Pressemitteilungen/EN/2021/bvg21-031.html

[5] https://www.bundesverfassungsgericht.de/SharedDocs/Downloads/DE/2021/03/rs20210324_1bvr265618.pdf

[6] Expertenrat für Klimafragen, Bericht zur Vorjahresschätzung der deutschen Treibhausgasemissionen für das Jahr 2020. Prüfung und Bewertung der Emissionsdaten gemäß § 12 Abs. 1 Bundes-Klimaschutzgesetz, 15 April 2021

[7] Kountouris, P., Gerbig, C., Rödenbeck, C., Karstens, U., Koch, T. F. and Heimann, M.: Atmospheric CO2 inversions on the mesoscale using data-driven prior uncertainties: quantification of the European terrestrial CO2 fluxes, Atmos. Chem. Phys., 18(4), 3047–3064, doi:10.5194/gmd-8-805-2015, 2018.

[8] Frey, M., Sha, M. K., Hase, F., Kiel, M., Blumenstock, T., Harig, R., Surawicz, G., Deutscher, N. M., Shiomi, K., Franklin, J. E., Bösch, H., Chen, J., Grutter, M., Ohyama, H., Sun, Y., Butz, A., Mengistu Tsidu, G., Ene, D., Wunch, D., Cao, Z., Garcia, O., Ramonet, M., Vogel, F., and Orphal, J.: Building the COllaborative Carbon Column Observing Network (COCCON): long-term stability and ensemble performance of the EM27/SUN Fourier transform spectrometer, Atmos. Meas. Tech., 12, 1513-1530, https://doi.org/10.5194/amt-12-1513-2019, 2019.

[9] Vogel, F. R., M. Frey, J. Staufer, F. Hase, G. Broquet, I. Xueref-Remy, F. Chevallier, et al. : XCO2 in an Emission Hot-Spot Region: the COCCON Paris Campaign 2015, Atmos. Chem. Phys., 3271–85, doi:10.5194/acp-19-3271-2019, 2019.

[10] Hase, F., M. Frey, T. Blumenstock, J. Groß, M. Kiel, R. Kohlhepp, G. Mengistu Tsidu, K. Schäfer, M. K. Sha, and J. Orphal: Application of Portable FTIR Spectrometers for Detecting Greenhouse Gas Emissions of the Major City Berlin, Atmospheric Measurement Techniques 8 (7): 3059–68. doi:10.5194/amt-8-3059-2015-supplement, 2015.

[11] Heinle, L. and Chen, J.: Automated enclosure and protection system for compact solar-tracking spectrometers, Atmos. Meas. Tech., 11, 2173-2185, https://doi.org/10.5194/amt-11-2173-2018, 2018.

[12] Kille, N., Chiu, R., Frey, M., Hase, F., Sha, M. K., Blumenstock, T., Hannigan, J.W., Orphal, J.W., Bon, D. and Volkamer, R.: Separation of methane emissions from agricultural and natural gas sources in the Colorado Front Range, Geophysical Research Letters, 46, https://doi.org/10.1029/2019GL082132, 2019.

[13] Krautwurst, S., K. Gerilowski, H. H. Jonsson, D. R. Thompson, R. W. Kolyer, L. T. Iraci, A. K. Thorpe, M. Horstjann, M. Eastwood, I. Leifer, S. A. Vigil, T. Krings, J. Borchardt, M. Buchwitz, M. M. Fladeland, J. P. Burrows and H. Bovensmann, Methane emissions from a Californian landfill, determined from airborne remote sensing and in situ measurements, Atmos. Meas. Tech., 10, 3429-3452, 2017.

[14] Krings, T., B. Neininger, K. Gerilowski, S. Krautwurst, M. Buchwitz, J. P. Burrows, C. Lindemann, T. Ruhtz, D. Schuettemeyer, and H. Bovensmann, Airborne remote sensing and in situ measurements

of atmospheric CO2 to quantify point source emissions, Atmos. Meas. Tech., 11, 721-739, https://doi.org/10.5194/amt-11-721-2018, 2018.

[15] ICOS Handbook https://www.icos-ri.eu/sites/default/files/2019-05/ICOS_handbook_2019.pdf

[16] Levin, I., Kromer, B., Schmidt, M., and Sartorius, H.: A novel approach for independent budgeting of fossil fuel CO2 over Europe by (CO2)-C-14 observations, Geophys Res Lett, 30, Artn 2194 Doi 10.1029/2003gl018477, 2003.

[17] Turnbull, J.C., Keller, E.D., Baisden, T., Brailsford, G., Bromley, T., Norris, M., and Zondervan, A., Atmospheric measurement of point source fossil CO2 emissions: Atmos. Chem. Phys., 14, 5001–5014, doi: 10.5194/acp-14-5001-2014, 2014.

[18] Petzold, A., V. Thouret, C. Gerbig, A. Zahn, C. A. M. Brenninkmeijer, M. Gallagher, M. Hermann, et al. 2015. “Global-Scale Atmosphere Monitoring by in-Service Aircraft – Current Achievements and Future Prospects of the European Research Infrastructure IAGOS.” Tellus B 67 (0): 13801. doi:10.5194/acp-7-4953-2007.

[19] Reuter, M., Buchwitz, M., Schneising, O., Krautwurst, S., O’Dell, C.W., Richter, A., Bovensmann, H., Burrows, J.P.: Towards monitoring localized CO2 emissions from space: co-located regional CO2 and NO2 enhancements observed by the OCO-2 and S5P satellites. Atmos. Chem. Phys. 19, 9371–9383. doi:10.5194/acp-19-9371-2019, 2019

[20] Copernicus CO2 Monitoring Mission https://www.esa.int/Our_Activities/Observing_the_Earth/Copernicus/Candidate_missions .

[21] Report for Mission Selection: CarbonSat , ESA SP-1330/1, June 2015, https://esamultimedia.esa.int/docs/EarthObservation/SP1330-1_CarbonSat.pdf .

[22] Ehret, G., Bousquet, P., Pierangelo, C., Alpers, M., Millet, B., Abshire, B. J, et al. (2017). MERLIN: A French-German Space Lidar Mission Dedicated to Atmospheric Methane. Remote Sensing, 9(10). doi:10.3390/rs9101052.

[23] Wunch, D., Toon, G. C., Blavier, J.-F. L., Washenfelder, R. A., Notholt, J., Connor, B. J., Griffith, D. W. T., Sherlock,V., and Wennberg, P. O.: The Total Carbon Column ObservingNetwork, Philos. Trans. R. Soc. A, 369, 2087–2112,doi:10.1098/rsta.2010.0240, 2011.

[24] Kretschmer R et al., 2013,Toward Assimilation of Observation-Derived Mixing Heights to Improve Atmospheric Tracer Transport Models, In Geophysical Monograph Series, 185–206, Washington, D. C., AGU, doi:10.1029/2012GM001255.

[25] D. Crisp et al., A Constellation Architecture For Monitoring Carbon Dioxide And Methane From Space, CEOS White Paper, 2018. http://ceos.org/document_management/Virtual_Constellations/ACC/Documents/CEOS_AC-VC_GHG_White_Paper_Publication_Draft2_20181111.pdf.

[26] Krings, T., B. Neininger, K. Gerilowski, S. Krautwurst, M. Buchwitz, J. P. Burrows, C. Lindemann, T. Ruhtz, D. Schuettemeyer, and H. Bovensmann, Airborne remote sensing and in situ measurements of atmospheric CO2 to quantify point source emissions, Atmos. Meas. Tech., 11, 721-739, https://doi.org/10.5194/amt-11-721-2018, 2018.

[27] Amediek, A., G. Ehret, A. Fix, M. Wirth, C. Büdenbender, M. Quatrevalet, C. Kiemle, and C. Gerbig, "CHARM-F — a new airborne integrated-path differential-absorption lidar for carbon dioxide and methane observations: measurement performance and quantification of strong point source emissions," Appl. Opt. 56, 5182-5197, doi:10.1364/AO.56.005182 (2017).

[28] ESA (2016). Sentinel-5 Precursor: ESA’s Atmospheric Chemistry and Pollution-Monitoring Mission. ESA SP-1332. European Space Agency, Noordwijk, the Netherlands. https://esamultimedia.esa.int/multimedia/publications/SP-1332/SP-1332.pdf

[29] ESA (2020). Sentinel-5: ESA's Polar-orbiting Atmospheric Composition Mission in Support of Copernicus Services. ESA SP-1336, European Space Agency, Noordwijk, the Netherlands. https://esamultimedia.esa.int/docs/EarthObservation/SP_1336_Sentinel-5_web.pdf

[30] Klausner, T., Mertens, M., Huntrieser, H., Galkowski, M., Kuhlmann, G., Baumann, R., Fiehn, A., Jöckel, P., Roiger, M.P.A.A., 2020. Urban greenhouse gas emissions from the Berlin area: A case study using airborne CO2 and CH4 in situ observations in summer 2018 1–24. doi:10.1525/journal.elementa.411

[31] Fiehn, A., Kostinek, J., Eckl, M., Klausner, T., Gałkowski, M., Chen, J., Gerbig, C., Röckmann, T., Maazallahi, H., Schmidt, M., Korbeń, P., Neçki, J., Jagoda, P., Wildmann, N., Mallaun, C., Bun, R., Nickl, A.-L., Jöckel, P., Fix, A., and Roiger, A.: Estimating CH4, CO2 and CO emissions from coal mining and industrial activities in the Upper Silesian Coal Basin using an aircraft-based mass balance approach, Atmos. Chem. Phys., 20, 12675–12695, https://doi.org/10.5194/acp-20-12675-2020,

[32] Wolff, Sebastian und Ehret, Gerhard und Kiemle, Christoph und Amediek, Axel und Quatrevalet, Mathieu und Wirth, Martin und Fix, Andreas, 2021: Determination of the emission rates of CO2 point sources with airborne lidar. AMT,14 (4), pages 2717-2736, doi: 10.5194/amt-14-2717-2021.

[33] Eldering, A., Taylor, T. E., O'Dell, C. W., and Pavlick, R.: The OCO-3 mission: measurement objectives and expected performance based on 1 year of simulated data, Atmos. Meas. Tech., 12, 2341-2370, https://doi.org/10.5194/amt-12-2341-2019, 2019.

[34] Kaminski, T., et al. (2013), The BETHY/JSBACH Carbon Cycle Data Assimilation System: experiences and challenges, *J. Geophys. Res. Biogeosci.*, 118, 1414– 1426, doi:10.1002/jgrg.20118, 2013.

[35] Kaminski, T., Scholze, M., Voßbeck, M., Knorr, W., Buchwitz, M., and Reuter, M.: Constraining a terrestrial biosphere model with remotely sensed atmospheric carbon dioxide, Remote Sens. Environ., 203, 109–124, 2017.

[36] Bousquet, Philippe und Pierangelo, Clémence und Bacour, Cédric und Marshall, Julia und Peylin, et al.(2018), Error Budget of the MEthane Remote LIdar missioN and Its Impact on the Uncertainties of the Global Methane Budget. JGR-A, 123 (20), pages 11766-11785, doi: 10.1029/2018JD028907.

Appendix A Detailed Description of Module M Activities

In the following, short descriptions of Modul M Workpackages, and their tasks, required input, foreseen output and deliverables for the individual workpackages are listed.

Module M is coordinated by Dr. Christoph Gerbig (MPI-BGC).

WP-M.1 Consolidation of experience

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

Participating partner: MPI-BGC, Dr. habil. Christoph Gerbig

The existing experiences with existing data assimilation with ICON and ICON-ART are combined with the experiences with flux inversions from the CarboScope Regional inversion system (CSR). Other research, e.g. with WRF-GHG and from the Copernicus services are included in the review.

Tasks: SWOT (Strengths, Weaknesses, Opportunities, Threats) Analysis, scientific performance tracking, evaluation of development opportunities

Input: Advice from experts in trace gas data assimilation and numerical weather prediction at DWD and KIT-IMK-ASF, and in inverse modelling of GHGs at MPI-BGC

Output: Reports on SWOT, performance indicators, development opportunities

Deliverables: D-M.1.1 SWOT [month o- 6] and updates at Milestones MS-M.2-5,

D-M.1.2 Report on performance indicators [month o-14] and updates at MS-M.3 and 5,

D-M.1.3 Report on opportunities for development [month o-51]

Scientists from relevant WPs will contribute

Used: as input to WP-M.11, Module V (WP-V.1-2)

WP-M.2 Evaluation of biogenic CO2 fluxes and anthropogenic CH4 emissions

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

To continuously provide information to be used as annex to the national GHG reporting (ITMS Module V), the existing CSR inversion system will be used initially for CH4. As biogenic CO2 fluxes from biospheric photosynthesis and respiration processes in Germany are larger than the anthropogenic emissions, and are subject to larger uncertainties, at this stage anthropogenic fluxes of CO2 are prescribed in the inversion. With the use of CAMS boundary conditions and ICOS data, a near-real-time inversion system is to be set up to provide sub-annual updates of GHG flux estimates. Should bias errors in CAMS GHG fields still prevent this, the global CarboScope model will be used to provide boundary conditions. Atmospheric observations provided by Module B, covering year n-1, will be used in the flux estimate that will be delivered around September of year n. The system will be continuously updated by utilising improvements developed within T2.3-6.

Tasks: are associated with the provision of annual updates of GHG flux estimates.

Input: ICOS atm. CO2 and CH4 data from Module B (WP-B.1, B.2, B.11, B.12), CO2 and CH4 boundary conditions from CAMS, prior fluxes from Module Q&S (WP-Q&S.2-6) (initially using VPRM and EDGAR-BP)

Output: Monthly maps and national balances of CH4 emissions and biogenic CO2 fluxes, annually updated

Deliverables: D-M.2.1-4 Top-down estimates for biogenic CO2 fluxes,

D-M.2.5-8 Top-down estimates for CH4 emissions

Used: as input to Module V (WP-V.1-2)

WP-M.3 Implementation of ICON meteorological fields in CSR

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

The CSR system uses the Lagrangian model STILT driven by meteorological fields (winds etc.) from the ECMWF IFS at a resolution of 0.25° × 0.25° (roughly consistent with the spatial resolution of IFS fields in 2006). The NWP system at DWD can provide met. fields from the ICON-EU nest at a much higher resolution (6.5 km). To improve on the Lagrangian transport these meteorological fields shall be implemented for use within STILT. This also enhances the comparability with the ICON-ART based GHG data assimilation when the CSR is used as a reference inversion.

Tasks: Selection of meteorological fields to be used by ICON for STILT transport simulations; Test simulations for CO2 to compare STILT-ICON and STILT-ECMWF with ICOS atmosphere observations; Implementation of operational transfer of the ICON meteorological fields.

Input: ICOS atm. CO2 data (WP-B.1), ICON meteorological fields

Output: CSR inversions using ICON meteorology.

Deliverables: D-M.3.1 Lagrangian Transport consistent with ICON for CSR [month o-15],

D-M.3.2 Performance assessment against ECMWF based STILT CO2 simulations [month o-21],

D-M.3.3 pre-operational use of ICON fields in CSR [month o-27]

Used: as input to WP-M.2.

WP-M.4 Improvement of vertical mixing

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

Participating partner: DWD, Dr. Linda Schlemmer

A significant limitation in inverse transport modelling of sources and sinks of greenhouse gases results from the necessary parameterisation of unresolved mixing processes (turbulence) in the atmospheric boundary layer, which leads to an inaccuracy of the vertical profiles of GHGs and in an inexact estimate of the height of the mixing layer (mixing height MH). Observation-based MHs can be derived from radio soundings (weather balloons), aircraft data (AMDAR), and from ceilometers or lidars.

So far, simulated MHs have been compared with observations from radiosondes, and, using Kriging interpolation to combine simulated and observed MHs, improved STILT simulations of atmospheric transport have been possible [24].

Within this WP, the massive data stream from the Ceilometer Network of the DWD with more than 150 stations will be used to derive MHs. In the STILT approach, those will be used to obtain optimized MH fields for use in STILT and thus in CSR inversions.

In the ICON approach, different MH definitions will be evaluated using observations. This will be done offline using output from ICON simulations. The most promising approaches will be implemented into the ICON model in order to compute MH online on the native ICON grid. Moreover, the distribution of GHGs within the mixed layer and MH will be used to further evaluate the PBL parameterization and its interplay with the shallow and deep convection scheme in ICON-ART. By comparing to observations, the modelling settings best suited for the greenhouse gas concentration modelling in 3D and time evolution as needed for the ITMS emission verification will be identified.

Tasks MPI-BGC: Optimization of the determination of MHs from ceilometer backscatter profiles using further data sets (AMDAR, radiosondes); Quantitative comparison of the mixing layer determined from ceilometer data with mixing layer heights diagnosed from ICON fields using a variety of approaches; Preparation of optimized MH based on ICON modelled and ceilometer derived MHs, Utilization of optimized MHs for GHG simulations with STILT-ICON and comparison with ICOS GHG observations, comparison with STILT-ICON transport simulations without optimized MHs; Comparison of impact in CSR inversion.

Tasks DWD: Exploring various methods to estimate MH and implement the most promising methods into ICON-ART; Identify the best configuration of the turbulent mixing, shallow and deep convection parameterizations, comparing with temperature and moisture observations as well as observed mixing heights, with uncertainty characterization for vertical mixing; Provision of an optimal setting of the vertical mixing scheme for GHG applications together with uncertainty characterization and recommendations concerning blacklisting or certain meteorological conditions (i.e., flagging of situations suitable or unsuitable for subsequent inversion estimation); Assessment of the technical developments for PBL modelling moving to kilometre-scale resolution: Advice concerning the choice of turbulence and convection scheme best suited to represent GHG transport at grey-zone resolution as well as the technical setup of a further refined inner nest.

Input: MH information from Ceilometer network, ICOS atm. GHG data (WP-B.1), aircraft in-situ profiles (WP-B.11)

Output: Improved vertical transport for CSR, improved MHs from ICON, provision of optimal setting of the vertical mixing scheme, flag for suitable/unsuitable meteorological conditions for subsequent inversion estimation.

Deliverables: D-M.4.1 Provision of offline ICON mixing heights [DWD, month o-15],

D-M.4.2 Assessment of vertical mixing uncertainty in ICON [DWD, month o-21],

D-M.4.3 Provision of online ICON mixing heights [DWD, month o-21],

D-M.4.4 Provision of observation-derived mixing heights [MPI-BGC, month o-21],

D-M.4.5 Evaluation of PBL parameterizations and model settings w.r.t. vertical mixing with MH observations [DWD, month o-39],

D-M.4.6 Evaluation of performance in STILT [MPI-BGC, month o-39],

D-M.4.7 Technical effort estimate and advice for modelling GHG transport at grey-zone resolution (= kilometre scale) [DWD, month o-39],

D-M.4.8 Evaluation of performance in CSR inversion [MPI-BGC, month o-51],

D-M.4.9 Evaluation of performance enhancement in ICON-ART [DWD, month o-51]

Used: as input to WP-M.2, WP-M.8-11

WP-M.5 Utilization of ICOS and IAGOS vertical profiles

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

The current CSR inversion system only uses concentrations measured at the top level of ICOS tall towers, and only during conditions when the boundary layer is well mixed (i.e. 11:00-16:00 LT). ICOS profile data from the tall towers principally contain valuable information on nocturnal fluxes from the temporal change of the profile during (e.g. CO2 increase as respired CO2 accumulates in the nocturnal stable boundary layer). Furthermore, IAGOS GHG data measured from commercial airliners provide high vertical resolution profiles up to and beyond the boundary layer, thus containing information on surface-atmosphere fluxes. This WP augments the CSR inversion system to utilize both these data streams.

Tasks: Implementation of separate respiration and photosynthesis in the inversion system; Adaptation of transport calculations for profiles; Comparison of nocturnal mixing layer heights derived from profile measurements with those from the transport model; Implementation of the observation operator for measurements of the integrated vertical profile within the nocturnal mixing layer; Evaluation of inversion results against standard inversion, calculation of a-posteriori uncertainties.

Input: ICOS atm. GHG profile data (WP-B.1), IAGOS profile data (WP-B.2), aircraft in-situ data (WP-B.9 - B.11)

Output: Augmentation of the inversion system to utilize full profile information provided by ICOS and IAGOS

Deliverables: D-M.5.1 Separate top-down estimates of respiration and photosynthesis [month o-27],

D-M.5.2 Evaluation of night-time MH [month o-33],

D-M.5.3 Integrated profile observation operator [month o-39],

D-M.5.4 Evaluation of performance against standard CRS inversion [month o-51]

Used: as input to WP-M.2.

WP-M.6 Simultaneous use of multiple species

Responsible partner: MPI-BGC, Dr. habil. Christoph Gerbig

The utilization of data streams of several greenhouse gases and associated trace gases in inverse modelling is expected to increase the reliability of estimated flux distributions through synergy effects. Those synergy effects result from similarities in emission patterns and in atmospheric transport for the different tracers. Prominent examples are the combination of atmospheric observations of CO2 and 14C-CO2 that allows for separation of biogenic from anthropogenic fluxes of CO2, and the use of Radon, which provides useful information on atmospheric mixing. Within this task, the capability to simultaneously assimilate observations of multiple species will be developed.

Tasks: Implementation of a radon exhalation model using soil moisture from ICON; Implementation of 14C-CO2 as additional data stream in the inversion system; Implementation of an emission model for CO2, CH4, N2O, 14C-CO2, CO and NOx, with quantification of a-priori errors (incl. correlations between tracers); Implementation of the simultaneous use of the tracers in the inversion, taking into consideration an adequate weighting of the different data density; initially limited to in-situ measurements; Test inversion and comparison with standard inversion, including a-posteriori uncertainties; Preparation of multi-species approach for the ICON-ART GHG assimilation system.

Input: ICOS atm. data for CO2, CH4, N2O, 14C-CO2, CO, NOx, and Radon (WP-B.1, B.2, B.11, B.13); GHG emissions and uncertainties from Module Q&S; soil 222Rn emission fields from Q&S.13;

Output: Multi-species inversion capability

Deliverables: D-M.6.1 Simulated radon fluxes for one year [month o-27],

D-M.6.2 CRS augmentation to use 14C-CO2 [month o-27],

D-M.6.3 CSR augmentation to use multi-species emissions [month o-33],

D-M.6.4 Multi-tracer implemented in CSR inversion [month o-39],

D-M.6.5 Evaluation of performance against standard CSR inversion [month o-51],

D-M.6.6 Quantified cost and benefit estimation for multi-species implementation in the ICON-ART system [month o-51]

Used: as research result for ITMS-M Phase 2

WP-M.7 Specification of the ICON forward model for ITMS

Responsible partner: KIT-IMK-ASF, Dr. Roland Ruhnke

DWD’s nonhydrostatic model system ICON (ICOsahedral Nonhydrostatic) is an online-coupled global to regional-scale modelling framework. The included Module ICON-ART (Aerosol and Reactive Trace gases) is designed for the simulation of the spatio-temporal evolution of aerosols and trace gases. ICON-ART-LAM is the limited area mode implementation, e.g., for Europe or Germany, which can be driven by external, e.g., CAMS concentration fields for trace gases at the boundary. Although GHGs have a long lifetime, for long-term monitoring purposes the chemical depletion has to be taken into account. For this, an altitude-spatial dependent lifetime-based approach being computationally cheap will be used via ART. In addition, by tagging the trace substances by source type (anthropogenic, biogenic) and source region, the contributions of individual source groups and regions can be distinguished and quantified. Extensive tagging allows for both sectorial disaggregation as well as separating emissions regionally. GHGs, passive tracers, and experiments with boundary conditions from Copernicus varying the grid and simulated model area, which are oriented on the operational NWP grids ICON-EU and ICON-D2, respectively, will allow to identify the optimal model setup. Performance optimization of the model system with respect to maximizing tagging capabilities as well as specification of number of affordable tags, grid resolution and model area is required in view of sensible computing power allocation and value added.

Experiments will be done with both ICON meteorology and CAMS meteorology as the boundary. Experiments will be repeated with increasing quality of Module Q&S a-priori fields. The quality can be accessed by comparing the forecasted concentrations with ICOS observations.

Tasks: Implementation and experiments with boundary conditions from ICON and CAMS, Development of optimal model setup w.r.t. resolution, area, tagging and computing efforts

Input: CAMS boundary conditions (chemistry and meteorology), ICON boundary conditions, at MilestonesQ&S1: hourly resolved flux fields (from Module Q&S)

Output: ICON-ART-LAM forward model specifications and ICON-ART-LAM tracer fields

Deliverables: D-M.7.1 First version of atmospheric forward model for ITMS [month o-12],

D-M.7.2 First report on comparison to observations [month o-12],

D-M.7.3 Second version of atmospheric forward model for ITMS [month o-18],

D-M.7.4 Second specification report, including optimal boundary condition implementation, [month o-18],

D-M.7.5 Third version of atmospheric forward model for ITMS [month o-30],

D-M.7.6 Third specification report covering optimal tagging and lifetime implementation, recommendations for area and resolution [month o-30],

D-M.7.7 Validation by comparison with observations [month o-36],

D-M.7.8 Final version of atmospheric forward model for ITMS [month o-45],

D-M.7.9 Final specification report on forward model [month o-48]

Used: as input for WP-M.8-11

WP-M.8 Development of initial GHG assimilation within ICON-ART

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

The aim is to develop a demonstrator for assimilating the CH4, CO2 observations (preparing also for N2O) from ICOS or comparable point observations in the ICON-ART-LAM system by adjusting concentration fields. Synergies with the meteorological data assimilation environment at DWD are to be used, as this is the key for successful operations of ITMS in the future.

Tasks: development of initial data assimilation and method testing for synthetic data, subsequently for CH4 and CO2 observations respectively: point data observation operator, blacklisting, bias correction, error covariances.

Input: ICON-ART-LAM forecast fields (from WP-M.7); ICON quality information (WP-M.4); quality controlled CH4 and CO2 in-situ observations from WP-B.1 and WP-B.2; selected validation data from Module B (WP-K.4)

Output: ICON-ART-LAM based ITMS concentration assimilation demonstrator, CH4, CO2 analysis fields, feedback statistics

Deliverables: D-M.8.1 Demonstrator for synthesis data assimilation of ICOS data [month o-15],

D-M.8.2 First ICOS CH4 data assimilation feedback statistics [month o-27],

D-M.8.3 Second ICOS CH4 data assimilation feedback statistics [month o-39],

D-M.8.4 Demonstrator for ICOS CO2 data assimilation [month o-39],

D-M.8.5 Third ICOS data assimilation feedback statistics [month o-48],

D-M.8.6: Report on performance of assimilation for CH4 and CO2 [month o-51]

Used: as input for WP-M.9-11

WP-M.9 Development of the ICON GHG satellite data assimilation

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

The initial GHG satellite data assimilation system within ICON-ART-LAM is developed, starting with CH4 satellite column assimilation of S5P data, preparing for MERLIN CH4 observations and CO2 satellite observations. The assimilation will provide optimized concentration fields.

Tasks: CH4 satellite data assimilation starting with synthetic data, proceeding to S5P, and preparing for MERLIN: observation operator, blacklisting, bias correction, model error covariances, obs. error covariances , comparison of analysis fields from CAMS, CHE and with /without satellite data assimilation monitoring of computing efforts

Input: ICON-ART-LAM forecast fields (from WP-M.7) and analysis fields (from WP-M.8), ICON quality information (WP-M.4); satellite observations from WP-B.3, WP-B.4, and synthetic data from WP-B.8; selected validation data from Module B (WP-K.4)

Output: CH4 analysis fields, feedback statistics, Comparison with CAMS, demonstrating performance of the ICON-ART-LAM based system

Deliverables: D-M.9.1 Demonstrator for synthetic GHG satellite data [month o-21],

D-M.9.2 Demonstrator of observation operator for S5P CH4 data[month o-27],

D-M.9.3 First Demonstrator of CH4 assimilation with ICON-ART-LAM [month o-39],

D-M.9.4 First S5P CH4 feedback statistics [month o-39],

D-M.9.5 Second version demonstrator of satellite CH4 assimilation with ICON-ART-LAM [month o-48],

D-M.9.6 Second version satellite CH4 feedback statistics [month o-48],

D-M.9.7 Report on CH4 satellite data assimilation [month o-51]

Used: as input for WP-M.10-12

WP-M.10 Development of the ICON-ART GHG inversion for flux estimation

Responsible partner: DWD, Prof. Roland Potthast

This Workpackage develops the initial ICON GHG inversion system with ICON-ART-LAM, preparing for delivery of a posteriori emission estimates. The system should use strong synergies with the meteorological data assimilation environment at DWD, as this is the key for successful operations of ITMS in future.

The atmospheric data assimilation of DWD employs both variational and ensemble data assimilation techniques. On the global scale, the ensemble-variational method EnVAR for the deterministic global ICON model is used. A global ensemble data assimilation is based on the localized ensemble transform Kalman filter LETKF, also creating initial conditions for the ICON ensemble prediction system. On the convective regional scale, for COSMO-D2 the 4D-LETKF is run operationally for COSMO-D2 and COSMO-D2-EPS. For ICON-ART, in cooperation with Karlsruhe Institute of Technology (KIT), DWD is currently developing an EnVAR based data assimilation based on aerosol optical depth (AOD) retrieved from MODIS satellite measurements to assimilation measurements relevant to Saharan dust and volcanic ash.

The development of the data assimilation for the “Integrated Greenhouse Gas Monitoring System” ITMS intends to rely on the experience of the operational atmospheric and aerosol related assimilation systems, using as far as possible synergies with the CSR inversion scheme and also from the Community Inversion Framework (CIF) of H2020 project VERIFY.

Tasks: Develop the algorithmic basis for GHG data assimilation within the data assimilation coding environment DACE of DWD, including the input/output and processing of GHG model fields within DACE, carry out and support the coding work to extend DACE and its EnVAR components GHG assimilation, develop the interfaces and observation operators to integrate the existing GHG estimation systems and their estimation results as measurements or components into the ICON-ART and its assimilation cycle, develop tools and basic cycling scripts for the above components to study the system within single assimilation steps, set up of test bed for synthetic inversions, test inversion system with perturbed CHE and CAMS analyses, test inversion system with ICON-ART-LAM analyses (specification of control vector, ensemble, time resolution, tags for CH4), monitor computing efforts, evaluate potential for assimilating the height of the mixing layer (as provided by WP-M.4)

Input: a-priori from WP-K.5, forecast and analyses fields from WP-M.7-9, mixing layer information from WP-M.4, selected validation data from Module B (WP-K.4) and Module Q&S (e.g., WP-Q&S.5)

Output: CH4 a posteriori emission fields and their uncertainty estimate

Deliverables: D-M.10.1 First CH4 core inversion step

[month o-15],

D-M.10.2 ICON-system test bed for EnVAR method development [month o-15],

D-M.10.3 Demonstrator of CH4 inversion with perturbed CHE and CAMS analyses [month o-27],

D-M.10.4 Demonstrator of inversion with sectorial segregation by ICON-ART-LAM [month o-33],

D-M.10.5 Status review and gap analysis of data assimilation system and capabilities, including evaluation of potential for mixing height assimilation [month o-39],

D-M.10.6 Demonstrator for CH4 and CO2 a posteriori flux estimates [month o-45],

D-M.10.7 Report on inversion specification and inversion results [month o-51]

Used: as input for WP-M.11

WP-M.11 Transfer to operations

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

To prepare the future operational ITMS service, the operational environment for the ICON GHG emission inversion system is built and gradually optimized with respect to computing resources. The (intermediate) results of WP-M.7, WP-M.8, WP-M.9, and WP-M.10 are implemented and linked. Performance measures, also relying on independent data, are implemented. Computing performance is monitored. The system should especially focus on using strong synergies with the operational environment at DWD.

Tasks: set up of the operational environment, transfer results of WP-M.7, WP-M.8, WP-M.9, WP-M.10 to an operational system, monitoring of computing efforts and performance, SWOT analysis of developing system.

Input: SWOT analysis (from WP-M.1); Module Q&S a-priori via WP-K.5, appropriate observation data from Module B via WP-K.4.; system components developed in WP-M.7-10

Output: Operational system demonstrator

Deliverables: D-M.11.1 Operational ITMS system architecture overview [month o-27], D-M.11.2 Demonstrator of overall system and SWOT analysis [month o-33],

D-M.11.3 Performance measures of system components at Milestone MS-M.3 [month o-39],

D-M.11.4 Performance evaluation of overall system [month o-48],

D-M.11.5 Report on operational system, procedures for components update, performance checks and maintenance [month o-51]

Used: as input to Module V (WP-V.1-2)

WP-M.12 OSSE for a urban scale observing system for anthropogenic CO2

Responsible partner: UHEI, Dr. Sanam Vardag

Metropolitan areas and individual cities are committed, so-called "non-state actors" in the Paris Climate Convention; they are organized in initiatives such as C40 or ICLEI. Especially for these cities, significant changes in fossil fuel CO2 (ffCO2) emissions are to be expected in the future. 14CO2 is the most direct tracer for observing the CO2ff concentration. The current ICOS class-1 atmosphere station network provides the background activity of 14CO2 for Germany and Europe, but it is not suitable for targeted monitoring of urban areas, as the ICOS stations explicitly avoid local anthropogenic source influences. Thus, in order to track CO2ff, additional observation networks adapted to the respective urban area are required.

The aim of this WP is to design cost-effective observation strategies for fossil CO2 emissions from German cities and metropolitan areas. In the proposed observing system simulation experiment (OSSE), the potential of different observation networks and sampling strategies to quantify CO2ff emissions and reduce uncertainty will be investigated and evaluated. This will be done by high-resolution inversion of realistic synthetic concentration data including a-priori errors and model data mismatch. The EU-funded projects CHE and RINGO are currently pursuing similar questions, but on a European scale and with relatively low spatial resolution, or as case studies, e.g. for Northern France and the Benelux countries. The model study proposed here should concentrate on German conurbations such as Berlin-Brandenburg, Rhine-Ruhr area, Rhine-Main-Neckar area, as well as Munich and Nuremberg. The results of this model study provide the basis for an efficient and cost-optimised future CO2ff observation network of conurbations in Germany.

Tasks: include high-resolution forward modelling for selected hotspot regions for one year using a modelling system that ensures synergy with other ITMS developments, either a variant of ICON-LAM-ART, or (if not feasible) existing systems such as WRF-GHG WRF-STILT or WRF-Flexpart (WP-M.7-10); Development of different hotspot-specific observation networks and sampling strategies; Inversion of the forward model concentrations "sampled" with different strategies for selected hotspots in Germany; Evaluation of the inversion results and evaluation of the sampling strategies.

Input: Input realistic spatio-temporal distribution of CO2 emissions at 1km spatial resolution (if possible, already from Module Q&S), verification data from WP-B.4, WP-B.6 and WP-B.10.

Output: Evaluation of observation strategies for fossil fuel related CO2 emissions from selected German cities or metropolitan areas

Deliverables: D-M.12.1 One year GHG simulations for selected hotspot regions [month o-24],

D-M.12.2 Definition of observing strategies to be evaluated [month o-27],

D-M.12.3 Inversions for each hotspot region [month o-30],

D-M.12.4 First evaluation of observation strategies for fossil fuel related CO2 emissions from targeted German cities or metropolitan areas [month o-36],

D-M.12.5 Final evaluation of observation strategies for fossil fuel related CO2 emissions from selected German cities or metropolitan areas [month o-48]

D-M.4.1

Used: as research result for ITMS Phase 2 (D-M.12.1, D-M.11.4)

WP-M.13 Data management and stewardship of operational data streams

Responsible partner: DWD, Dr. Andrea Kaiser-Weiss

Tasks: Main tasks are the quality monitoring and further development of the measurement data streams operationally required in the ITMS, the organisation of the operational interfaces and data flow of the auxiliary quantities, the troubleshooting and support of related Module B and Module M activities, the management of disk space and computer resources as well as quality assurance incl. version control, traceable documentation and archiving of the underlying material. Critical issues from an operational perspective are analysed and improved.

Input: data streams from Module B provided by WP-K.4 as in pre-operational use by Module M (WP-M.2 and WP-M.8-11), data from Module Q&S provided by WP-K.5.

Output: Data, document and software management system suitable for ITMS future operations (D-M.13.1-M.13.4).

Deliverables: D-M.13.1: Plan for data management, document management, software management [month o-9],

D-M.13.2: Report on data, document and software management [month o-27],

D-M.13.3: Reporting on data, software, documentation management and issues from an operational perspective [month o-39],

D-M.13.4. Documentation and recommendations for future operations [month o-51]

Appendix B Detailed Description of Module B_I Activities

In the following, short descriptions of Module B_I Workpackages, and their tasks, required input, foreseen output and deliverables for the individual workpackages are listed.

Module B_I is coordinated by Dr. Heinrich Bovensmann (UBre).

WP-B_I.1 Observation Data Synthesis and Coordination

Responsible partner: **UBre**, Dr. Heinrich Bovensmann, Dr. Michael Buchwitz

Main focus of this activity is to ensure that observational data from Module B are fit for purpose for the usage within ITMS in terms of interfaces and data quality. This will include the harmonisation of interfaces, the coordination of campaigns (called WPs within B_II) as well as the identification of observational gaps and initiation of steps towards closing critical observational gaps by improving the observation system in the future. This work package will also support Module K (overall ITMS Coordination), will organise regular meetings of Module B partners as well as perform the reporting including regular reporting on Module B milestones and deliverables in cooperation with the Module B work package leads.

Tasks: Harmonisation of interfaces with Module M and Q&S, identification of observational gaps and approaches to close critical gaps, identification of data weaknesses and initiation of corrective actions, stimulating exchange between Module B work packages, stimulating and coordinating campaign activities, stimulating interaction within ITMS and external w.r.t. future development of the observation system, tracking of progress, risks, deliverables and milestones across Module B ork packages in support of Module K.

Input: ITMS requirements from Module M and Q&S on data format, interfaces, data quality needs as well as information from Module B WPs on data characteristics, formats and availability.

Output: Yearly *Observation Data Synthesis Report* (D-B_I.1.1 -.4), Inputs to IMTS reporting and benchmarking

Used: Across Module M, B, K, and Q&S

Deliverables:

D-B_I.1.1: Observation Data Synthesis Report [month: 12]

D-B_I.1.2: Observation Data Synthesis Report [month: 24]

D-B_I.1.3: Observation Data Synthesis Report [month: 35]

D-B_I.1.4: Observation Data Synthesis Report [month: 48]

WP-B_I.2 Provision of In-situ Concentration Data from ICOS and IAGOS Tailored to ITMS Applications and Extension of ICOS Tall Tower Measurements

Responsible partner: **DWD**, Dr. Dagmar Kubistin, Dr. Jennifer Müller-Williams

Participating partners: **MPI-BGC**, Dr. habil. Christoph Gerbig (IAGOS in-kind)

This WP supports the provision and QA of in-situ concentration data from ICOS and IAGOS. This includes for IAGOS greenhouse gases (CO_2, CH_4, partly N_2O) as well as reactive gases (O_3, CO, NO_x, NO_y) along flight corridors. For ICOS it will include, beside the continuous monitoring of atmospheric greenhouse gas (GHG) concentrations (CO_2, CH_4, CO, N_2O, ^{14}C) at the atmospheric stations (mostly tall tower), the upgrade of selected atmospheric tall towers with NO_x measurement capabilities to provide an additional tracer sensitive to CO_2ff sources. ICOS data are provided for all 9 tall tower stations by DWD, 2 mountain stations and one marine site by UBA (Fig. 8) and IAGOS data for all IAGOS starts and landings at German airports with the GHG package on board.

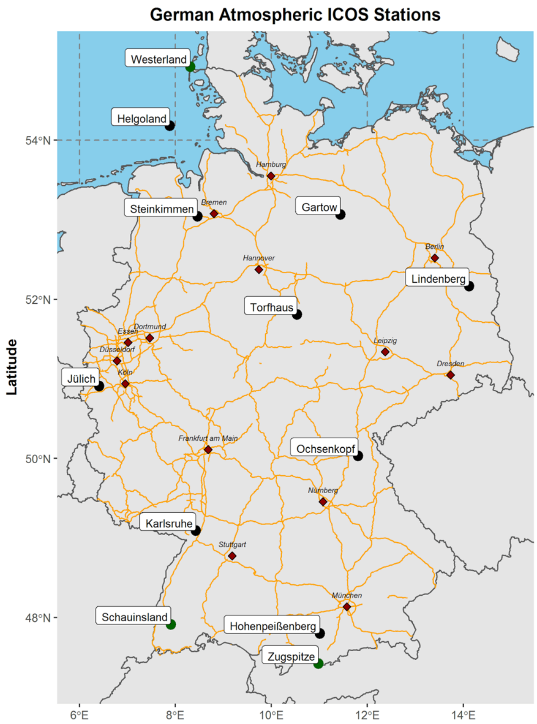

Figure 8: ICOS-D tall tower stations.

Tasks: Provision of ICOS data, provision of IAGOS data, support to QA and provision of data uncertainty, support to data usage w.r.t. inverse modelling, implementation of NO_x (based on modified CAPS systems), measurements at selected ICOS-D atmospheric tall towers (planned are 5 towers), operational provision of quality-controlled NO_x data in NRT, operational provision of measured concentration ratios classified according to air mass origin (trajectories), creation of continuous tracer-based datasets for CO_2ff, derived from emission ratios, provision of multi-tracer measurements for operational inverse modelling.

Input: Operational data from ICOS and IAGOS research infrastructure

Output: Quality controlled ICOS and IAGOS data (D-B_I.2.1-4)

Used: As input to Module M

Deliverables:

D-B_I.2.1: ICOS and IAGOS first data delivery (CO_2, CH_4) [month: 12]

D-B_I.2.2: ICOS and IAGOS second data delivery (CO_2, CH_4, N_2O) [month: 24]

D-B_I.2.3: ICOS and IAGOS third data delivery (CO_2, CH_4, N_2O, NO_x) [month: 35]

D-B_I.2.4: ICOS and IAGOS final data delivery and data delivery and quality report [month: 48]

Note: The provision of QA controlled standard ICOS (CO_2, CH_4, CO, N_2O, 14C) data is an in-kind contribution of DWD. The provision of QA controlled IAGOS (CO_2, CH_4, O_3, CO, NO_x, NO_y) data is an in-kind contribution from members of the IAGOS-AISBL via MPI-BGC. Both provisions are granted for free and associated work is provided by DWD and MPI-BGC in-kind with no financial requests to ITMS project. Just the NO_x measurement infrastructure and data flow at ICOS towers are set-up in the framework of ITMS and needed funding is requested for the researcher.

WP-B_I.3 Provision of Ground-based In-situ Data from ICOS and TERENO Ecosystem Sites

Responsible partner: **Thünen Institute**, Dr. Christian Brümmer, Dr. Frederik Schrader

Participating partners: **KIT-IMK-IFU**, PD Dr. Ralf Kiese

This WP supports the provision of in-situ concentration and flux data from ecosystem sites from ICOS and TERENO stations for process characterisation and modelling within Module Q&S. This will include fluxes for CO_2, H_2O and CH_4, N_2O where available from eddy covariance measurements as well as related ecosystem parameters [15]. Ecosystem data (ICOS, TERENO) are provided for the existing stations and when available for new stations (stations see Fig. 9) via the ICOS and TERENO data portals.

Figure 9: ICOS-D and TERENO ecosystem stations.

Tasks: Compilation and provision of in-situ concentration and flux data, support to QA, support to data usage for ICOS and TERENO ecosystem sites w.r.t. process studies (Module Q&S), support data access via TERENO data portal

Input: Data from ecosystems sites

Output: Quality controlled in-situ and flux data (D-B_I.3.1-3.4)

Used: As input to Module M and Module Q&S

Deliverables:

D-B_I.3.1: ICOS and TERENO flux data: first data delivery [month: 12]

D-B_I.3.2: ICOS and TERENO flux data: second data delivery [month: 24]

D-B_I.3.3: ICOS and TERENO flux data: third data delivery [month: 35]

D-B_I.3.4: ICOS and TERENO flux data: data delivery and quality report [month: 48]

Note: The compilation and provision of QA controlled ecosystem flux data from common ICOS and TERENO stations is an in-kind contribution of Thünen and KIT-IMK-IFU.

WP-B_I.4 XCH_4 S5P Satellite Data Tailored for ITMS Applications

Responsible partner: **UBre**, Dr. Michael Buchwitz, Dr. Oliver Schneising-Weigel

Atmospheric XCH_4 fields from satellite remote sensing are planned to be assimilated by ITMS. This WP focusses on the optimisation of S5P XCH_4 for applications at and below the national scale. It will provide quality controlled data with minimised systematic errors at high spatial resolution and dense coverage for Germany and surrounding areas. Currently, two S5P XCH_4 retrieval algorithms and corresponding data products exist: the operational Copernicus product and a scientific product generated by UBre using the WFMD algorithm. The UBre WFMD product has already been used to quantify methane emissions of major gas and oil fields (mostly outside Europe). Initial validation results at sparse TCCON sites indicate similar quality of both products but regional spatial patterns show significant differences in terms of XCH_4 values and coverage. The coverage of the WFMD product is typically better, which is important for ITMS applications. In this WP detailed comparisons of the latest data products will be carried out focussing on Germany and surrounding countries and it will be investigated to what extent the WFMD product can be further improved for ITMS applications. This includes optimized quality filtering and bias correction to enhance the yield (coverage) and to minimize biases. This also includes detailed uncertainty characterization and validation (TCCON, COCCON when available) but also detailed comparisons with the latest version of the operational product. In case issues are identified with the operational product, feedback will be given with the potential to improve also the quality of the operational product. As S5P data is available from early 2018 onwards, this WP will generate a 5-year data set optimized for central Europe. The two data sets (WFMD and operational) will be analysed in detail, for example, with respect to spatial patterns and trends. It will also be investigated to what extent emission information can be derived using, for example, mass balance methods applied to regions showing locally elevated methane, i.e., to methane emission hotspots. In case of issues (e.g., sparseness, biases, large uncertainties etc.) it will be aimed at to further improve the data quality as relevant for ITMS applications. It will also be investigated to what extend changes in terms of atmospheric concentrations and / or emissions can be detected and quantified. If successful, this approach will then be used to verify changes in emissions determined by ITMS.

Tasks: Evaluate existing S5P XCH_4 data products (operational and WFMD) with respect to IMTS needs. Optimise S5P XCH_4 retrievals for ITMS applications to generate an appropriate data product (high yield, low bias, low scatter) for Germany and surrounding countries, where local emission signals are typically weaker compared to regions outside Europe (e.g., oil and gas fields in Turkmenistan and the US), where emission information has already been successfully derived. Use of the improved algorithm to generate a 5-year S5P XCH_4 data set (2018-2022) optimized for IMTS. Validation of this data set by comparison with ground-based observations (TCCON, COCCON). Analysis of this data set w.r.t. spatial patterns and trends. Application of the mass balance approach to this data set to obtain emission information for selected emission hot spots. Definition of data product content and format (with Module M) including supporting the preparation of observation operators for total column XCH_4 data (with Module M).

Input: S5P Level 1 (from Copernicus/ESA), S5P Level 2 (from Copernicus/ESA), S5P XCH_4 WFMD algorithm, TCCON (COCCON when available via B_II)

Output: Quality controlled XCH_4 data tailored to ITMS needs for Module M and time series analysis of changes in CH_4 concentrations and emissions (D-B_I.4.1 - 3)

Used: As input to Module M

Deliverables:

D-B_I.4.1: S5P XCH_4 data interface and data quality report, incl. test data [month: 24]

D-B_I.4.2: S5P XCH_4 optimised data product [month: 35]

D-B_I.4.3: S5P XCH_4 ensemble product and trend assessment [month: 48]

WP-B_I.5 XCO_2 Satellite Data Tailored for ITMS Applications

Responsible partner: **UBre**, Dr. Michael Buchwitz, Dr. Maximilian Reuter

Atmospheric XCO_2 fields from satellite remote sensing are planned to be assimilated by ITMS. Currently only OCO-3 on ISS (successful launch 5/2019) [25] delivers images of XCO_2 over selected regions (e.g., coal fired power plants, cities) for selected times. From 2025/26 onwards, the European COPERNICUS CO2M mission is planned to provide such data regularly and with much better coverage. The focus of this WP is to exploit existing space-based observations of XCO_2 images (from OCO-3) and to optimally prepare for CO2M, also providing XCO_2 images. This WP focus on the use and optimisation of OCO-3 XCO_2 for applications at and below the national scale. It will provide quality controlled data with minimised systematic errors for high spatial resolution. This will be achieved by detailed analysis of OCO-3 XCO_2 data products. For this application it is important to not only use the existing OCO-3 XCO_2 data product from NASA (an activity already ongoing via a DWD funded PhD project) but also to generate an independent OCO-3 XCO_2 data product from the OCO-3 radiance spectra as only this permits to have full control over product generation, its interpretation (including error analysis) and potential optimization for the envisaged ITMS applications. For this purpose, the UBre FOCAL algorithm will be used, which has initially been developed for OCO-2 but is currently also used for GOSAT and GOSAT-2. This provides the possibility to improve data product quality and the option to generate an ensemble of products, e.g., obtained by varying relevant retrieval algorithm parameters, which can be used to characterize uncertainties introduced by the retrieval technique. Achieving highest possible data quality, robustness and detailed data product characterization is important for ITMS applications. FOCAL is also a candidate Level 1 to Level 2 algorithm for operational processing of CO2M data at EUMETSAT. EUMETSAT plans to generate simulated CO2M Level 1 and Level 2 product files and UBre will have access to these global data set. Within this WP it is planned to use a subset of this data set to generate appropriate simulated CO2M Level 2 test data sets as input for Module M in addition to OCO-3 XCO_2 images.

Tasks: Adjust the existing UBre retrieval algorithm FOCAL for OCO-3 XCO_2 retrieval and use it to generate XCO_2 images for selected anthropogenic CO_2 emission targets such as power plants and cities. The new data product will be evaluated and optimized for ITMS applications (in Module M). This includes detailed error analysis, validation (TCCON, COCCON) and comparisons with other satellite XCO_2 products (e.g., GOSAT-2). A key aspect will be the evaluation of the two OCO-3 XCO_2 data products, the NASA product and the FOCAL product, with respect to ITMS needs (Module M) in particular for Germany and its surroundings. This also includes to investigate the information content with respect to CO_2 emissions by studying aspects related to the identification of emission plumes and application of approaches such as mass balance methods to estimated emissions. In addition to these actually measured XCO_2 data sets also simulated CO2M data sets will be generated and provided (to Module M) to support preparation of usage of CO2M data within ITMS.

Input: OCO-3 Level 1 and Level 2 **Snapshot Area Maps** data (available from NASA), FOCAL algorithm, simulated CO2M products (available from EUMETSAT), GOSAT-2, TCCON and COCCON XCO_2 products.

Output: XCO_2 data from OCO-3 **Snapshot Area Maps** for selected regions in Germany and surrounding countries and simulated CO2M data (D-B_**I**.5.1-3)

Used: As input to Module M

Deliverables:

D-B_I.5.1: XCO_2 (OCO-3) data quality and CO2M prelim. data interface report [month: 24]

D-B_I.5.2: XCO_2 optimised product (OCO-3) incl. validation [month: 35]

D-B_I.5.3: XCO_2 final data delivery (incl. synthetic test data CO2M) and quality report [month: 48]

WP-B_I.6 Satellite Data on Fossil Fuel Tracer CO and NO_2 Tailored for ITMS Applications

Responsible partner: **UBre**, Dr. Andreas Richter, Dr. Oliver Schneising-Weigel

CO_2 emission from fossil fuel combustion are accompanied by emissions of CO and NO_x, the latter quickly converting to NO_2. The ratio of CO and NO_x to CO_2 depends on the fuel and the combustion efficiency and temperature. CO and NO_x (NO_2) can therefore be used as tracers to identify different combustion processes and to distinguish between different combustion sources. Data assimilation of these tracers has the potential to help separating biogenic fluxes from fossil fuel CO_2 emissions. If emission factors are sufficiently well known, then derived emissions of these tracers (as obtained via inverse modelling) can also be used to obtain information on CO_2 emissions. However, such applications require appropriate information on atmospheric CO and NO_2 concentrations. Neither the operational tropospheric NO_2 product nor the operational CO column product are optimised for ITMS applications. The focus of this WP is therefore to generate appropriate NO_2 and CO data products from S5P focussing on Germany and surrounding countries. This includes detailed error characterization, validation and comparisons with other existing satellite-derived NO_2 and CO including the operational S5P data products. To establish concentration ratios relative to CO2, model data (Modul M) or - where colocations are available - satellite-derived XCO_2 products (from WP-B_I.5) will be used. Concentration ratios will be analysed to answer the questions how far they can be linked to emission ratios.

Tasks: Evaluate the data quality of XCO and tropospheric NO_2 from S5P w.r.t. ITMS needs, optimise retrievals for high spatial resolution applications up to the national scale, minimise small scale systematic errors by retrieval algorithm improvements, e.g. using up-to-date high resolution a-priori knowledge, perform error characterisation, define data product content and format, support the preparation of observation operators, produce and provide quality controlled XCO and tropospheric NO_2 from S5P tailored to ITMS applications, calculate and analyse concentration ratios.

Input: S5P Level 1, S5P Level 2 (available from Copernicus/ESA); CO and NO_2 retrieval algorithms (available at IUP UBre)

Output: Quality controlled XCO and tropospheric NO_2 data tailored to ITMS needs, computation and analysis of concentration ratios and comparisons with emission ratios (D-B_I.6.1 - D-B_I.6.3)

Used: As input to Module M, comparison with emission ratios from Module Q&S, research result for ITMS Phase 2

Deliverables:

D-B_I.6.1: S5P tropospheric NO_2 and XCO data interface and data quality report [month: 24]

D-B_I.6.2: S5P optimised tropospheric NO_2 and XCO data quality report [month: 35]

D-B_I.6.3: Report on tropospheric NO_2 and XCO product analysis (incl. concentration ratios) [month: 48]

WP-B_I.7 Land Surface Satellite Data Tailored for ITMS Applications

Responsible partner: **MPI-BGC**, Dr. Gregory Duveiller, Dr. Martin Jung, Prof. Dr. Markus Reichstein

Up-to-date spatially explicit CO_2 fluxes between the ecosystems and the atmosphere ("gridded fluxes") at high spatial (< 10 km, goal 1 km) and temporal (hourly) are an important basis of ITMS. They can be derived by a data-driven bottom-up approach. With machine learning, eddy covariance measurements, climate data and satellite data can be mapped onto spatially distributed CO_2 biosphere fluxes, an important input ITMS-M and to be generated in WP3 of the ITMS-Q&S_I Module. The present work package in Module ITMS-B_I is to establish a flexible and operationalizable workflow for acquiring and processing the relevant satellite based land surface data for the estimating high spatial resolution, hourly biogenic CO_2 fluxes through the integration of machine learning of satellite data and ecosystem measurements by ITMS-Q&S_I WP3. The request for funding here has a focus on the development of a semi-operational workflow for the acquisition and processing of satellite data, as this operational aspect is not funded otherwise.

Tasks: Merge, harmonize process, and quality control of satellite data from various complementary sources (e.g., MODIS, VIIRS, SEVIRI, Sentinel-3) around eddy covariance measurement stations and spatially-temporally explicit for the regional domain; development and application of product and region-specific quality control of satellite data, adaptation/development/application of specific algorithms for filling gaps in the satellite data, regular re-processing and temporal updates of satellite data; setup, operationalization, and maintenance of the software and data environment.

Input: MODIS, VIIRS, SEVIRI and Sentinel-3 satellite data

Output: Space-time fields of various satellite data for the regional domain as well as extracted time series for ecosystem stations which are representative for German climate and geo-ecological conditions (European and other temperate zone stations) (D-B_I.7.1-3)

Used: As input to Module ITMS-Q&S_I WP3

Deliverables:

D-B_I.7.1: Preliminary land surface satellite data delivery [month: 17]

D-B_I.7.2: Land surface satellite data delivery and quality report [month: 35]

D-B_I.7.3: Final land surface satellite data delivery and quality report [month: 48]

WP-B_I.8 XCH_4 MERLIN Preparation for ITMS Applications

Responsible partner: **DLR-IPA**, Dr. Andreas Fix, Dr. Christoph Kiemle

With the upcoming CH_4 lidar satellite mission MERLIN (launch planned 2027), XCH_4 data will become available with smaller systematic errors as from passive remote sensing system like S5P. The very small footprint (~100 m) reduces sensitivity to cloud cover, and the day and night measurement capability are further key assets for providing complementary data to S5P and S5 XCH_4. In the long term, both types of XCH_4 data are planned to be assimilated into the ITMS. Consequently, this WP focuses on the preparation of MERLIN XCH_4 retrieval for applications at and below national scale. It will provide synthetic XCH_4 MERLIN data and its error characterisation. It will also provide data to investigate the potential of deriving two pieces of information (above and below boundary layer columns using the Earth surface and cloud tops as the reflecting targets) on XCH_4 in the lower troposphere. The methane flux estimates (Level-4 data in the MERLIN nomenclature) are explicitly excluded from the scope of the mission ([22], [36]). Since sophisticated inversion systems are required to retrieve the fluxes and infer the sources and sinks from the Level-2 data products, it is consensus that research institutions operating such models should address this task. Exactly this would be the goal usage of XCH_4 from MERLIN within ITMS and requires respective funding as not funded elsewhere. A specifically tailored product with a high flexibility to feed a German ITMS is not to be expected from the operational MERLIN processing operated by CNES. For this reason, a custom-made scientific Level-2 processor from the Level-1 products focusing on the area of interest needs to be developed within this project. In order to do so, recent and upcoming campaign data (provided as an in-kind contribution) from the airborne MERLIN demonstrator CHARM-F will be made available to provide test data sets. Currently, CHARM-F is the only system in Europe to provide MERLIN-like data products before launch. Of utmost importance is a detailed characterization of random and systematic errors. Due to the nature of the IPDA lidar technique, the random error of a single measurement can be reduced or increased by appropriate averaging at the expense of spatial resolution. The optimum balance between resolution and error for best results within Module M will be subject to detailed analysis.

Tasks: Develop retrieval algorithms for MERLIN XCH_4, perform error characterisation of the data product according to the needs of Module M, define data product content and format (with Module M), support preparation of observation operator for MERLN XCH_4 data (with Module M), produce and provide simulated MERLIN XCH_4 test data product, investigate profile information content using synthetic MERLIN data and CHARM-F campaign data

Input: Synthetic MERLIN Level 1 data, CHARM-F data from CoMet campaign

Output: Quality controlled synthetic MERLIN XCH_4 data tailored to ITMS needs (D-B_I.8.1-3)

Used: As input to Module M (CHARM-F data for verification) and preparation of Phase 2 data use

Deliverables:

D-B_I.8.1: MERLIN XCH4 data interface and synthetic data quality report [month: 24]

D-B_I.8.2: MERLIN XCH4 test data delivery [month: 35]

D-B_I.8.3: MERLIN XCH4 synthetic data delivery and quality report [month: 48]

Appendix C Detailed Description of Module Q&S _I Activities

In the following, short descriptions of Module Q&S_I Workpackages, and their tasks, required input, foreseen output and deliverables for the individual workpackages are listed.

Module Q&S_I is coordinated by Prof. Klaus Butterbach-Bahl (KIT-IMK-IFU).

WP1 GHG emissions by the sectors industry, transport, energy and waste

Responsible partner: UBA, Dirk Günther / Dr. Christian Mielke

In this WP the Umweltbundesamt will work on spatio-temporal downscaling of anthropogenic emissions from the sectors industry, transport, energy and waste.

Tasks: Identifying the essential parameters (activity data and emission factors) driving spatio-temporal patterns. Assessment of uncertainties (incl. assessment of co-variations). Development of emission maps for the years 2005 to 2020, which however will still be coarse (e.g. monthly at best) and not fully comply with spatio-temporal demands of the ITMS system. Comparison and harmonization of spatiotemporal scaled emission fields with other data sources (TNO Bottom-up emission estimates for anthropogenic CO_2 and with other data sources (e.g. TNO co-emitted tracers at 5 km)). Development of temporal activity fields for various source categories. Operationalisation and integration of data in ITMS system.

Input: Information on sectoral GHG sources (e.g. industry, landfills, etc.) as used for NIR, other EU-datasets (e.g. TNO).

Output: Spatio-temporal downscaled of sectorial GHG emission fields for industrial processes, households, energy generation and waste management

Deliverables:

D-Q&S_I.1.1	first data delivery	[month: 12, o-15]
D-Q&S_I.1.2	second data delivery	[month: 30, o-33]
D-Q&S_I.1.3	Operationalisation of data flow towards ITMS	[month: 36, o-39]

and updates at MS-Q&S_I

Used: Coarse a-priori emission fields for the industry, energy, household, transport and waste sectors for Modules ITMS-M (anthropogenic GHG sources) and ITMS-V, interpretation of campaign data by ITMS-B.

WP2 GHG fluxes for agricultural and forest sectors

Responsible partner: Thünen (TI), Dr. Christian Brümmer

In this WP Thünen Institute delivers spatial downscaled GHG National Inventory Reporting data (NIR) for the sectors agriculture, forestry and land use (AFOLU).

Tasks: Delivery of spatial downscaled CO_2, CH_4 and N_2O emission fields based on national UNFCCC reporting according to the “Nationalen Inventarbericht”, thereby differentiating between the various source categories such as livestock systems, direct soil emissions, indirect emissions and emissions due to landuse change.

Input: Data from National Inventory Reporting (NIR) on GHG emissions from AFOLU (GasEM), statistics on fertilizer use and agricultural management, national forest inventory data, livestock systems information incl. manure management schemes

Output: Dynamic database system on AFOLU GHG emissions for ITMS, coarse information on agricultural and forest management based on the results of an evaluation of existing data protection guidelines

Deliverables:

D-Q&S_I.2.1 first data delivery [month: 18, o-21]

D-Q&S_I.2.2 second data delivery and seamless integration of dataflow in ITMS [month: 48, o-51]

Used: input for ITMS-Q&S_I.4 and for comparison with ITMS-M, interpretation of campaign data by ITMS-B

WP3 Biogenic CO_2 fluxes

Responsible partner: MPI-BGC, Dr. Gregory Duveiller

Set-up of a flexible and operational workflow to estimate hourly biogenic CO_2 fluxes at high spatio-temporal resolution on basis of the integration of machine learning, satellite data and measurements of CO_2 fluxes and supplementary parameters at eddy co-variance sites in Germany. This will serve as a prior for the inversion activities of the ITMS-M module. This work leverages on the long expertise of the MPI-BGC group related to the FLUXCOM initiative (www.fluxcom.org).

Tasks: Consolidation of all necessary input information for training the machine learning methodology into a structured database. Aggregation of information and development of a suitable data structure allowing for machine learning. Production of emission fields of biogenic CO_2 fluxes based on the calibrated algorithms.

Input: Datasets of land surface satellite products specifically tailored for ITMS (ITMS-B_I.WP7). Meteorological gridded data and eddy covariance site data; Ancillary information from ITMS-Q&S_I.WP2.

Output: Provisioning of structured database for machine learning. First version of algorithms tested for limited dataset. First data delivery of estimated land biogenic CO2 fluxes.

Deliverables:

D-Q&S_I.3.1 First data delivery [month: 18, o-21]

D-Q&S_I.3.2 Final data delivery, seamless integration of dataflow in ITMS [month: 45/48, o-48/51]

Used: Input for ITMS-M.2 and ITMS-M.5 for cross validation.

WP4 Biogeochemical modeling of ecosystem GHG exchange

Responsible partner: KIT-IMK-IFU, Prof. Dr. Klaus Butterbach-Bahl

This WP will provide high spatio-temporal emission/deposition fields for CO_2, N_2O, and CH_4.

Tasks: This WP provides high spatio-temporal emission/deposition fields for CO_2, N_2O, and CH_4 for all major terrestrial ecosystem types (forest, arable land, grassland, wetlands). In this WP the relevant input and activity databases will be developed in cooperation with WPQ&S.3, information synthesized and made available for modelling at regional and national scale. Test dataset from ICOS, TERENO and other sites will be used for model testing and for assessing structural and parametric model uncertainties. Based on simplified assumptions on activity data (land and forest management) first GHG inventories will be calculated and a suitable input-output data structure for ITMS will be developed.

Input: Harmonized data from the GHG observational network ICOS/TERENO and other long-term observational sites (ITMS-B workpackages); advanced datasets on processes and GHG fluxes as supposed to be delivered by ITMS-Q&S_II. Activity data by ITMS-Q&S_I.2.1 and _I2.2.

Output: Site validation database for GHG (CO_2, CH_4, N_2O) fluxes from agriculture (crops & grassland), forestry and wetlands and regional activity database linked to models. Tested biogeochemical models with assessed structural and parametric uncertainty documented. First coarse a-priori emission fields for ecosystem CO_2, N_2O, and CH_4 fluxes

Deliverables:

D-Q&S_I.4.1 Model validation site scale [month: 12, o-15]

D-Q&S_I.4.2 Data flow scheme for ITMS [month: 30, o-33] D-
Q&S_I.4.3 Coarse regional emission fields [month: 36, o-39]

D-Q&S_I.4.4 Seamless dataflow from BGC model to ITMS [month: 45/48, o-48/51]

Used: Used by ITMS-M.5 and first a-priori terrestrial ecosystem GHG flux fields.

Appendix D Detailed Description of Module K Activities

In the following, short descriptions of Module K Workpackages, and their tasks, required input, foreseen output and deliverables for the individual workpackages are listed.

Module K is coordinated by Dr. Andrea Kaiser-Weiss and Dr. Christian Plaß-Dülmer (DWD).

WP-K.1 Communication and Meeting planning

Responsible partner: **MPI-BGC**

Participating partners: **DWD**, **UBre**, **KIT-IMK-IFU**

<u>*Tasks:*</u> Communication within the project is planned carefully at the beginning of the project (*Task 1*), facilitated by a setup of a convenient online communication tool, data exchange tool and webpage (*Task 2*) and organization of meetings and telecons (*Task 3*). *Task 4* concerns: tracking of progress of deliverables, many of which are the output of one Workpackage as well as the input of another Workpackage, risks and bottlenecks in achieving Milestones, progress of the partners and issue solving. Project communication is structured according to the Module Milestones and the WP Deliverables. Module K structures the communication around each MS with timetables and assigned responsibilities, risk-analysis, an alert system in case of delays or problems (traffic light system), and organizes a regular communication within the participating WPs. Where needed, specific MS-related meetings are realized.

<u>*Input*</u>: work plans and updates from modules ITMS-M, ITMS-B_I, ITMS-B_II, ITMS-Q&S_I, ITMS-Q&S_II, ITMS-V

<u>*Output:*</u> Online Project communication, organization of regular meetings and telecons with Coordination Group, Steering Group and Advisory group, organization of project meetings and General Meetings (D-K.1.1-11)

Deliverables [ITMS-K month/ overall ITMS o-month](responsible partners):

D-K.1.1: Communication and meeting plan, including regular telecons [month: 3/o-6] (DWD)

D-K.1.2: Internal online project communication and data exchange tools [month: 3/o-6] (MPI-BGC)

D-K.1.3: Core Kick-Off meeting [1/o-4] (MPI-BGC),

D-K.1.4: ITMS first General Meeting [14/o-17] (DWD)

D-K.1.5: First benchmark meeting [month: 18/o-22 (MPI-BGC)

D-K.1.6: ITMS second General Meeting [26/o-29] (DWD)

D-K.1.7: Second benchmark meeting [month: 31/o-34] (MPI-BGC)

D-K.1.8: ITMS third General Meeting [38/o-41] (DWD)

D-K.1.9: Third benchmark meeting [month: 43/o-46] (MPI-BGC)

D-K.1.10: Final General Meeting [month: 48/o-51] (DWD)

D-K.1.11: Risk analysis, an alert system in case of delays or problems (traffic light system), updated as needed, at least at the General Meetings (DWD)

WP-K.2 Project Reporting

Responsible partner: **DWD**

Participating partners: **MPI-BGC**

<u>*Tasks*</u> include all aspects of administrative management and regular progress reporting, facilitating public relations by listing achievements in user interaction, publications, press releases, and reports and updating the webpage. The work is structured in three tasks: *Task 1*: Traceability Matrix Design;

Task 2: achievement listing concerning data and model (interim-) products, their status and further development potentials; *Task 3*: formal project reporting.

Input: updates from Modules M, B, Q&S, V

Output: Project reporting (D-K.2.1-4)

Deliverables:

D-K.2.1: First Progress report incl. deliverable status and conceptual design of Traceability Matrix [month: 12/o-15] (DWD)

D-K.2.2: Second Progress report incl. deliverable status first consolidated Traceability Matrix [month: 24/o-27] (MPI-BGC)

D-K.2.3: Third Progress report draft incl. deliverable status updated Traceability Matrix [month: 36/o-39] (DWD)

D-K.2.4: Final report including deliverable status and updated Traceability Matrix [month: 48/o-51] (MPI-BGC)

WP-K.3 Benchmarking and Planning for Phase 2

Responsible partner: **DWD**

Participating partners: **MPI-BGC**, **UBre**, **KIT-IMK-IFU**

Tasks: Benchmarking will be built on K.1 and K.2, and uses the overarching milestones (ITMS-MS) to evaluate the corresponding achievements of the project and the effectiveness of cooperation and communication. Lessons learned in each benchmarking step are used to improve the coordination process. An important benchmarking associated with ITMS-MS 3 will analyse the status of the ITMS and the recommendations and needs for Phase 2. The Traceability Matrix (from Task K.1) will be applied for progress monitoring, as well for planning appropriately for Phase 2.

Input: updates from Modules M, B, Q&S, V, Traceability matrix design from WP K.2

Output: Filled traceability Matrix, benchmarking results, recommendations for Phase 2 (D-K.3.1-4)

Deliverables:

D-K.3.1: Applied Traceability Matrix and updates at GMs [month: 13/o-16, month: 25/o-28, month: 32/o-35] (DWD)

D-K.3.2: Milestone achievement evaluation [month: 17/o-20, month: 30/o-33, month: 42/o-45] (MPI-BGC)

D-K.3.3: Benchmarking reporting [month: 19/o-22, month: 32/o-35, month: 43/o-46] (DWD)

D-K.3.4: Recommendations for Phase 2 [month: 21/o-24, month: 33/o-36, month: 39/o-42] (MPI-BGC)

WP-K.4 Modules ITMS-B observation data provision for use by other Modules

Responsible partner: **UBre**

Tasks: The observation data flow will be provided and tracked according to project requirements, focussing on coverage, quality, timeliness, format specification and issue communication. Observational gaps will be identified in collaboration with Modules B_I and B_II as well as measures to close observational gaps will be initiated. Contributions from Modules B_I and B_II to overall progress, delivery status and ITMS-B benchmarks will be tracked.

Input: updates from Modules B_I and B via WP-B.0

Output: Modules B_I and B_II data provision management (D-K.4.1-4)

Deliverables:

D-K.4.1: Data flow from and to ITMS-B_I, regularly updated [month: 14/o-17, month: 26/o-29, month: 38/o-41, month: 48/o-51] (UBre)

D-K.4.2: Data flow from and to ITMS-B_II, regularly updated [month: 14/o-17, month: 26/o-29, month: 38/o-41, month: 48/o-51] (UBre)

D-K.4.3: Internal user requirements and observational gaps, regularly updated [month: 7/o-10, month: 17/o-20, month: 29/o-32, month: 41/o-44] (UBre)

D-K.4.4: Module milestones and issue tracing concerning Modules B_I and B_II, regularly updated [month: 9/o-12, month: 19/o-22, month: 32/o-35, month: 43/o-46] (UBre)

WP-K.5 Modules ITMS-Q&S bottom-up flux data provision for use by other Modules

Responsible partner: **KIT-IMK-IFU**

Tasks: The bottom-up flux data will be provided from ITMS-Q&S_I and ITMS-Q&S_II and tracked according to (project internal) user requirements, focussing on coverage, quality, timeliness, grid specification and issue communication. Data gaps will be identified in collaboration with Modules Q&S_I and Q&S_II and measures to close data gaps will be initiated. Contributions from Modul Q&S_I and Q&S_II to overall progress and benchmarks will be tracked.

Input: updates from Modules Q&S_I and Q&S_II

Output: Modules Q&S_I and Q&S_II data provision management (D-K.5.1-4)

Deliverables:

D-K.5.1: Bottom-up flux data provision from Q&S_I, regularly updated [month: 14/o-17, month: 26/o-29, month: 38/o-41, month: 48/o-51] (KIT-IMK-IFU)

D-K.5.2: Bottom-up flux data provision from Q&S_II, regularly updated [month: 14/o-17, month: 26/o-29, month: 38/o-41, month: 48/o-51] (KIT-IMK-IFU)

D-K.5.3: Synthesis report on internal user requirements, identification of research gaps and detailed definition of required future work (all WPs) [month: 7/o-10, month: 17/o-20, month: 29/o-32, month: 41/o-44] (KIT-IMK-IFU)

D-K.5.4: Synthesis report on Q&S_I and Q&S_II activities and progress, milestone and issue tracking [month: 9/o-12, month: 19/o-22, month: 32/o-35, month: 43/o-46] (KIT-IMK-IFU)

Appendix E: Acronyms and Abbreviations

AFOLU	Agriculture, Forestry and Other Land Use
AMDAR	Aircraft Meteorological Data Relay
B	Module B (Greenhouse gas observational data sets for ITMS)
BMBF	Bundesministeriums für Bildung und Forschung
BMEL	Bundesministeriums für Ernährung und Landwirtschaft
BMU	Bundesministerium für Umwelt, Naturschutz und nukleare Sicherheit
BMVI	Bundesministerium für Verkehr und digitale Infrastruktur
CAMS	Copernicus Atmosphere Monitoring Service
CMSAF	EUMETSAT Climate Monitoring Satellite Application Facility
CCDAS	Carbon Cycle Data Assimilation System
CCI	Climate Change Initiative
CHARM-F	CH_4 Airborne Remote Monitoring - Flugzeug
CHE	H2020 project: CO_2 Human Emissions
CH_4	Methane
COCCON	Collaborative Carbon Column Observing Network (FTIR)
CoMet	Carbon Dioxide and Methane Mission
Copernicus	Erdbeobachtungsprogramm Copernicus von EU und ESA
CO	Carbon monoxide
CO_2	Carbon dioxide
CO2M	CO_2 Monitoring Mission, a high priority COPERNICUS mission
CSR	CarboScope Regional
C3S	Copernicus Climate Change Service
D-	Deliverable
DKK	Deutsches Klimakonsortium
DLR	Deutsches Zentrum für Luft- und Raumfahrt
DWD	Deutscher Wetterdienst
EC measurements	Eddy Covariance measurements
EDGAR	Emission Database for Global Atmospheric Research
EDGAR-BP	Data of BP Statistical Review of World Energy used by EDGAR emission calculation
ESA	European Space Agency

FFDAS	Fossil Fuel Data Assimilation System
FTIR	Fourier-transform Infrared Spectrometers
FZJ	Forschungszentrum Jülich
GA	General Assembly
GasEM	Greenhouse gas inventory model to calculate emissions from agriculture
GFZ	Helmholtz-Zentrum Potsdam–Deutsches GeoForschungsZentrum
GHG	Greenhouse gas
GOSAT-2	Greenhouse Gases Observing Satellite 2 (IBUKI 2)
GRETA	Gridding Emission Tool for ArcGIS (UBA Software für Deutschland-Karten zu Luftschadstoff-Daten)
IAGOS	Integration of Routine Aircraft Measurements into a Global Observing System
IG3IS	Integrated Global Greenhouse Gas Information System
ICON	Icosahedral Nonhydrostatic Model (numerical weather prediction model of DWD)
ICON-ART	ICON Module for trace gases („Aerosols and Reactive Trace Gases“) – here intended to use for passive tracer transport
ICON-EU	DWD's regional ICON-EU nest which covers whole Europe with a grid spacing of 6.5 km
ICOS	Integrated Carbon Observation System
ICOS-D	ICOS National Network Germany
ICOS RI	Integrated Carbon Observing System Research Infrastructure
ICOS STK	ICOS tower in Steinkimmen
IPCC	Intergovernmental Panel on Climate Change
ITMS	Integriertes Treibhausgas-Monitoringsystem
IUP	Institut für Umweltphysik
K	Module K (Coordination)
KIT	Karlsruher Institut für Technologie
KIT-IMK-ASF	Institut für Meteorologie und Klimaforschung - Atmosphärische Spurengase und Fernerkundung des KIT
KIT-IMK-IFU	Institut für Meteorologie und Klimaforschung, Atmosphärische Umweltforschung des KIT
KIT-IMK-TRO	Institut für Meteorologie und Klimaforschung, Department Troposphärenforschung des KIT

KML	Keyhole Markup Language file format to use display data in an Earth browser such as Google Earth
LANDSAT	Earth Observation Satellites of NASA
Landscape-DNDC	Landscape-DeNitrification-DeComposition
LAM	Limited Area Mode
LPJ	Lund-Potsdam-Jena Dynamic Global Vegetation Model
LULUCF	Land Use, Land-use Change and Forestry
MAMAP	Methane Airborne Mapper
MERLIN	Methane Remote Sensing LIDAR Mission (German-French satellite mission)
M	Module M (Atmospheric Models & Inverse Methods)
MH	Mixing height
MODIS	Moderate Resolution Imaging Spectroradiometer by NASA
MPI	Max-Planck-Institut
MRV	Monitoring, reporting, verification
MS	Milestone
MVS	Monitoring & Verification Support systems
NDACC	Network for the Detection of Atmospheric Composition Change
NDC	Nationally Determined Contribution
NGO	Non-governmental organisation
NIR	National Inventory Reports
NO_2	Nitrogen dioxide
NWP	Numerical Weather Prediction
N_2O	Nitrous oxide
OCO-3	Orbiting Carbon Observatory-3
OSSE	Observing System Simulation Experiment
PM	Person month
PT	Projektträger
Q&S	Module Q&S (Sources and Sinks of Greenhouse Gases)
R-	Identified Risk
RINGO	Research, Infrastructure, Needs, Gaps and Overlaps; this is coordination and support action which funded by EU under H2020
S2	Sentinel-2 Satellite

S5P	Sentinel-5 Precursor satellite
STILT	Stochastic Time Inverted Lagrangian Transport
SWOT	Strengths, Weaknesses, Opportunites, Threats
TCCON	Total Carbon Column Observing Network
TERENO	Terrestrial Environmental Observatories (Helmholtz)
UBA	Umweltbundesamt
UFZ	Helmholtz-Zentrum für Umweltforschung GmbH
UNFCCC	United Nations Framework Convention on Climate Change
V	Module V (User interactions)
VERIFY	H2020 project: Observation-based system for monitoring and verification of greenhouse gases
VIIRS	Visible Infrared Imaging Radiometer Suite
VPRM	Vegetation Photosynthesis Respiration Model
VTT	Virtual tall tower
WMO	World Meteorological Organisation
WP	Workpackage
WRF-GHG	Weather Research and Forecasting model coupled with Greenhouse Gas Modules
XCH4	Column concentration of CH_4
XCO	Column concentration of CO
XCO2	Column concentration of CO_2