



CO₂
Human
Emissions

Progress report on
service element
requirements for
uncertainty
representation

Marko Scholze et al.

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CO₂ Human Emissions

D5.7 Progress report on service element requirements for uncertainty representation

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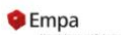


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1 Executive Summary

This deliverable documents the progress on characterising the main building blocks for representing uncertainty in an integrated anthropogenic CO₂ emissions monitoring system. All components of this CHE Prototype are considered here to provide a consolidated view on the characterization of uncertainties. The individual components themselves are discussed in their respective (progress) reports: Observations in D5.1, emissions and transport models in D5.3, inversion / data assimilation methodology in D5.5 and D5.9 provides a synthesis of these building blocks for an end-to-end prototype system. The focus of this report is first to list the uncertainty components of the individual building blocks for the prototype and how they contribute to the overall posterior uncertainty estimations, second to identify tools and metrics to evaluate and benchmark the posterior uncertainty estimates of the prototype, and third to identify the immediate development needs of the prototype with respect to the uncertainty representation as well as longer term research priorities together with an estimate of the required efforts. The overall posterior uncertainty estimate of the CHE prototype arises from uncertainties in the prior data, the model uncertainty, uncertainties in the observations as well as from the ability of the inversion / data assimilation to correctly represent the posterior uncertainty given the uncertainties of the before listed ingredients. An important aspect for the development of the CHE prototype is to identify the research needs for the near-term (next 3-4 year) development steps. This report lists these immediate development needs with an estimate of the required effort for the prototype with respect to the uncertainty representation in Table 3. It also provides a high-level overview of research priorities beyond the near-term development needs (Table 4). The report also emphasises the importance of benchmarking and evaluating the posterior uncertainty estimates of the prototype system. This aspect of the report will be extended for in the final version.

2 Introduction of the Building Block

2.1 Background

The CHE prototype aims at building a system to monitor the exchange of CO₂ and potentially other important man-made greenhouse gases like CH₄ between the Earth surface and the atmosphere with the use of observations (mostly in the atmosphere), models and prior information including the specification of their uncertainties. The system is designed to support the Paris Agreement and follows the directive of the EC as described by the Task Forces on CO₂ (Pinty et al., 2017). The general rationale and strategy for the CHE prototype is provided in D5.9, stemming from the discussions in the first WP5 workshop (Reading, 25-26 September 2019). The main challenges are addressed with the following recommendations:

- Multi-scale approach to monitor emissions from point sources (power stations or industrial facilities), cities and countries using different model domains from global, regional to local and model resolutions (e.g. from 25km to 100m).
- Multi-species approach to detect and attribute the observed atmospheric signal to specific sources/sinks (e.g. natural and anthropogenic emissions with sectorial distribution).
- Multi-stream approach to support different applications and users with a near-real time stream focusing on shorter synoptic timescales designed to provide early warnings and giving feedback to data producers, and a re-analysis stream that uses consolidated quality-controlled data, products and models with their associated uncertainties to estimate trends.

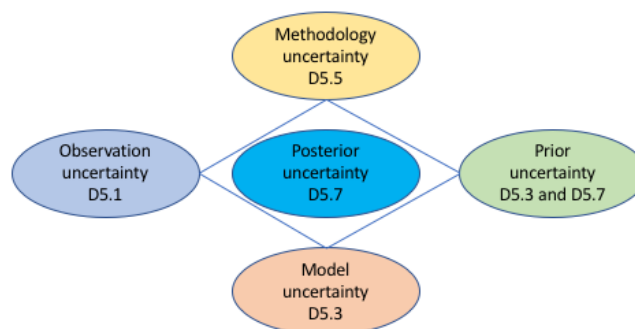


Figure 1: Building blocks of the CHE prototype with associated uncertainties and the specific deliverable reports associated with the specific building blocks.

This report covers the ingredients required for a robust representation of uncertainties in the building blocks of the CHE prototype including the prior, observation, model and methodological uncertainties (see Figure 1 and Table 1). A key focus of the report is on the derivation of posterior uncertainty and the validation of those uncertainty estimates, to assess the accuracy of the CO₂ monitoring system.

Aspects of uncertainty include, but are not limited to, prior uncertainty, transport model uncertainty, observation uncertainty (see deliverable D5.1 for more details), and posterior uncertainty. The correct representation and attribution of each uncertainty component is essential to construct an accurate operational CO₂ monitoring system. This report outlines these aspects of uncertainty and expands on two methodological different systems to quantify the theoretical posterior uncertainty. Furthermore, it focuses on details of benchmarking/validation activities, which can be used for assessing the accuracy of posterior uncertainties.

2.1.1 Prior Uncertainty

The prior uncertainty will be used to inform the assimilation system, which in turn will provide a posterior error reduction, which needs to be validated using independent observations (see D5.1 for more details on independent observations). Depending on the methodology the prior uncertainty takes on different forms. In a direct estimation of CO₂ fluxes by atmospheric transport inversion (in the following referred to as inversions) the prior uncertainty consists of spatio-temporal mapping of error statistics in the flux components that contribute to the atmospheric CO₂ concentration observations.

Prior flux uncertainties will be based on the available knowledge from state-of-the-art bottom-up inventories and terrestrial ecosystem models. However, given the level of uncertainty in those estimates, further adjustments for the prescribed prior error covariance matrix will be needed. In particular, flux error correlations are poorly known in current bottom-up inventories (see D3.2 and D3.3 for more details on this aspect of uncertainty) and models (e.g. Chevallier *et al.*, 2012).

In the case of process model optimisation (by estimating model process parameters but also model state variables and initial and boundary conditions) in a comprehensive data assimilation system (in the following referred to as data assimilation) the prior uncertainty enters the system as uncertainty on the parameters to be optimised, the so-called parametric uncertainty (see also Scholze *et al.*, 2012). These prior parameter uncertainties are usually derived from literature studies, field-scale measurements (e.g. in the case of the terrestrial biosphere), databases (e.g. plant trait database), or plausible assumptions. This approach does not require prescribed spatio-temporal error correlations in the prior flux field. The process models help to specify the uncertainty structure. The a priori assumption here is that there are no error correlations among the process parameters.

In summary, the prior flux uncertainty consists of:

- Spatio-temporal mapping of the uncertainty in the biogenic and anthropogenic fluxes.
- Process uncertainty and missing processes in the biogenic and anthropogenic models.
- Both mapping and process uncertainty related to other fluxes (e.g. biomass burning).
- Proxy information uncertainty, relevant to proxy observations (e.g. nightlights, co-emitted traces, radiocarbon).

D3.3 presents fossil fuel emissions and their uncertainties per sector on spatio-temporal maps and D3.2 presents net biospheric fluxes with uncertainties for use as prior information in the direct estimation of fossil fuel CO₂ fluxes by atmospheric inversions.

2.1.2 Model Uncertainty

Another important component for the representation of uncertainty in the CHE prototype is the transport model error, which forms part of the overall prior uncertainty.

In addition to the transport model (that acts as the observation operator linking the emissions to the atmospheric concentrations) uncertainty any other model included as an observation operator in the modelling chain in the CHE prototype adds to the overall model uncertainty. In the case of a data assimilation system these are the fossil fuel emissions model but also the terrestrial carbon cycle model.

The model (transport as well as other process models) uncertainty consists of:

- Uncertainty in the model input data, e.g. meteorological fields (from a reanalysis product or from an operational NWP system) for offline models.
- Structural uncertainty in the physics and parameterisation of model processes, including missing processes (e.g. atmospheric transport).
- Systematic model biases.

2.1.3 Observation Uncertainty

Observations and their uncertainties must also be considered, both observations used in the inversion or data assimilation but also observations used for the validation of the posterior fluxes, are key components as well. The details of the observation uncertainty (including the CO₂M satellite observations) that enter the inversion or data assimilation system are described in D5.1.

In short, the observation uncertainty consists of:

- Systematic and random error statistics of all observations.
- Model uncertainty (incl. models to derive higher level products, i.e. retrieval algorithms to derive column CO₂ measurements from radiances).
- The representation error, which occurs because of coarse resolution model trajectories being compared to point or finer resolution (satellite footprint) observations or mismatch in the spatio-temporal representation in the model.

2.1.4 Methodological / Posterior Uncertainty

Finally, the methodological error arises essentially from the ability of the chosen methodology to adequately represent the posterior uncertainty, an issue which is discussed in more detail in Section 4.

Table 1 : Uncertainty components and state of knowledge of them in an anthropogenic CO₂ inversion / data assimilation system

Component	Maturity	Representation	Example
Prior biogenic flux estimates or terrestrial ecosystem model process parameters	Medium - Considered in research. Accurate quantification requires further research.	Statistical approaches (multi-model spread or model comparison with observations) or literature assessment (e.g. trait database)	Chevallier <i>et al.</i> 2012
Prior anthropogenic flux estimates or fossil fuel emission model process parameters	Medium - Considered in research. Accurate quantification requires further research.	Rough estimates with little/no sector/country consideration; first attempts to get sub-annual, grid-cell based	Choulga <i>et al.</i> in prep.
Initial conditions (i. e. atmospheric 3D CO ₂ field, state of terrestrial ecosystems)	Poor to medium - Some research. State of knowledge is insufficient to be used in CHE prototype.	Statistical approaches (multi-model spread or model comparison with observations).	Chen <i>et al.</i> 2019
Model processes (physics, biogeochemistry)	Poor - Little or no research. Requires substantial research for use in CHE prototype.	Typically not considered directly, included by inflation of observation uncertainty.	McNorton <i>et al.</i> submitted
Meteorological conditions	Poor to medium - Some research. State of knowledge is insufficient to be used in CHE prototype.	Typically not considered directly, included by inflation of observation uncertainty.	McNorton <i>et al.</i> submitted
Observations	Good - In-situ data well characterised in current research. Medium - Bias problems with remotely sensed CO ₂ data	Reasonably good knowledge of in-situ observation accuracy, medium knowledge of remotely sensed XCO ₂ .	Connor <i>et al.</i> 2016
Representation error	Poor to medium - Some research. State of knowledge is insufficient to be used in CHE prototype.	Typically not considered directly, included by inflation of observation uncertainty (Less relevant with higher resolution).	Agusti-Panareda <i>et al.</i> 2019
Methodological error	Medium - Considered in research. Accurate quantification requires further research.	Typically not considered so far.	Trudinger <i>et al.</i> , 2007

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverables

The objective of this deliverable is to provide a progress report on requirements for representing the different sources of uncertainties in the localisation of CO₂ surface emission sources and the methods to reliably represent uncertainties and their variability with geographical, temporal and environmental conditions. This progress report will be updated following the results of respective tasks in WPs 1-3 related to the uncertainty representation. It will form the basis for the deliverable D5.8 'Final report on the service element requirements for the uncertainty representation'.

In the following sections the guiding principles for the uncertainty components are laid out followed by a more detailed consideration for the prior emissions and transport model components. Two hypothetical examples for posterior uncertainty estimation are provided. Finally, priorities for implementation by 2023 and for longer term research needs are outlined in Sections 4 and 5.

2.2.2 Work performed in this deliverable

Consultation with the partners involved with the respective tasks in WPs 1-3 and synthesis of this work with ESA-funded projects as well as literature on carbon cycle.

2.2.3 Deviations and counter measures

Not applicable.

3 Uncertainty Components of the CHE Prototype

3.1 Principles for the uncertainty components in the CHE prototype

The end product of the CHE prototype will consist not only of the flux estimates, but also posterior uncertainties, which will be validated using independent observations, for example flux towers, with the same consideration for errors such as the representation error.

There are multi-options for representation of the process/mapping prior uncertainty within a proposed prototype these include:

- Deriving statistics of prior variables vs. observation comparisons
- Multi-model for the transport component (e.g. Offline CTMs and Online NWP)
- Multi-model for the biogenic component (e.g. different photosynthesis and respiration schemes)
- Perturbed-flux inventory for the anthropogenic component (e.g. based on log-normal uncertainties)
- Multi-physics in the transport (e.g. convection)
- Perturbed-physics in the transport (e.g. Stochastically perturbed parameterisation tendencies)
- Multi-resolution for the representation component (e.g. comparing 1km resolution with 9km transport model)

The guiding principles for setting up a multi-model, multi-stream prototype are as follows:

- Modelling groups are required to use a consistent prior uncertainty, which is used in the derivation of posterior uncertainties. These include formulating the prior error correlation structures, or similar prior uncertainty for aggregated regions.

- The derivation/approximation of posterior uncertainties must also be consistent between assimilations.
- The benchmarking should consist of the evaluation of multiple aspects of posterior uncertainty (and beyond just concentration data as currently done in atmospheric transport inversions), i.e. evaluation of the uncertainty in fluxes, parameters and any other proxy information.

As mentioned in 2.1.3 the observational uncertainty is discussed in more detail in the deliverable report D5.1.

3.2 Uncertainty estimates for the prior emissions component

The 2006 IPCC guidelines, with 2019 refinements, outline the methodology by which anthropogenic emission uncertainties can be calculated based on emission factors and activity data for multiple sectors (70+). These uncertainties calculated at the national scale can be applied to gridded emission maps from EDGAR v4.3.2. Uncertainties are calculated dependent on the statistical development of a nation, with countries either being classified as having well (WDS) or less (LDS) developed statistical systems. Currently monthly uncertainty calculations are derived using the following steps (see Figure 2):

- The emission factor and activity data uncertainties are first combined for each IPCC activity preserving non-symmetrical upper and lower limits. This method accounts for only the most common fuel type per each activity, i.e. for aviation – Jet Kerosene, for railways – Diesel, for shipping – composition of 80% Diesel and 20% Residual Fuel Oil, and for road/off-road transport the most typical emission factor uncertainty is used (not fuel type, recommendation of IPCC2006).
- The original IPCC sectors are grouped into 20 EDGAR sectors following the error propagation methodology. Systematic underestimation is corrected following Frey (2003), with Monte Carlo approach comparisons if the uncertainty half-range is within the 100-230% range.
- All annual uncertainties are calculated with lower and upper bounds, which are then used to generate assumed log-normal uncertainty distributions. This prevents a probability distribution function with negative emissions from being constructed. The methodology, which follows that of IPCC (2006), calculates a geometric mean (which can be estimated based upon the arithmetic mean and arithmetic standard deviation) and a geometric standard deviation.
- If the lower uncertainty range $\geq 50\%$ then methodology outlined by Frey (2003) is applied to ensure the lower PDF range does not fall below 100%. Following this method, the decrease in the lower uncertainty range causes an approximately symmetric relative increase in the upper uncertainty range.
- The 20 EDGAR sectors are then combined further into 7 sectors following the error propagation method. This is done to reduce the size of the control vector within the CHE prototype. The grouped sectors are determined based on similarities in:
 - Activity type (point sources, 3D field, etc.)
 - Knowledge of the activity (uncertainty value)
 - Geographical distribution (e.g. over urban areas only)
 - Emissions of CO₂ co-emitting species (e.g. CH₄, CO, NO₂).

- Monthly uncertainties are calculated using an iterative approach, which is based on the methodology used to generate annual uncertainties (Figure 2). Estimates are derived using monthly emission budgets and annual prior uncertainties. These underestimate the monthly variability of emissions and need to be inflated proportionally to the error propagation method used for annual and summed monthly values. The Inflation step is repeated until the change in inflation value is ≤ 0.01 .
- The calculated mean and standard deviation of the log-normal distribution can then be used for inverse modelling and emission perturbations, assuming the lower and upper uncertainty bounds are 2.5th and 97.5th percentiles, respectively, of the 95 percent probability range.

The derived uncertainties are country and sector specific, with global values provided in D5.3. Further details of the derivation of annual and monthly uncertainties will be described in an upcoming manuscript (Choulga *et al.*, in prep). Currently, these calculations provide an uncorrelated prior uncertainty. Further work should aim to develop spatially and temporally correlated uncertainties and uncertainties at a high temporal resolution (<monthly).

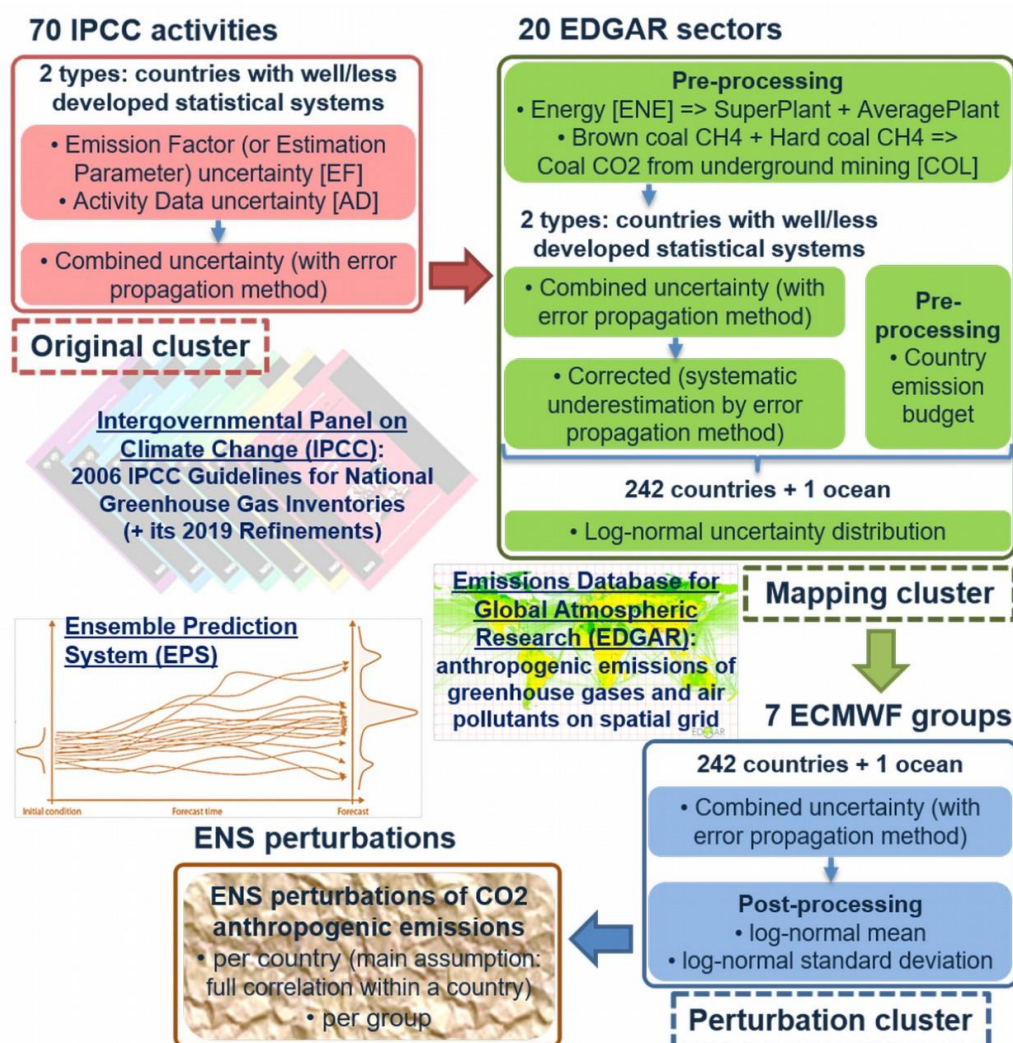


Figure 2: Schematic of methodology used to derive national annual and monthly uncertainties from activity and emission factor data through to a log-normal uncertainty distribution for 7 sectors per country.

3.3 Uncertainty estimates for the transport model component

The representation of uncertainty in atmospheric transport models is essential for estimating accurate posterior information within an inversion system. Uncertainties that are present in either offline, online or both offline and online models include those relating to:

- The initial 3D CO₂ model field.
- The initial meteorological conditions.
- The model physics relating to advection, convection and diffusion.
- Numerical uncertainty.
- The model representativeness.

In addition to these, within an earth system modelling context, uncertainties in meteorological variables can feedback on biogenic, or even modelled anthropogenic, fluxes.

Uncertainties in the initial conditions can occur from uncertainties in the observations used to derive the analysis fields. For numerical weather prediction (NWP), it is typically too computationally costly to calculate the analysis uncertainty, but the uncertainty can be represented using ensemble-based data assimilation approaches (such as the ensemble Kalman filter) or through an ensemble of data assimilations (EDA). These methods provide an ensemble of initial conditions based on prior and observational uncertainties and have successfully been used operationally within the NWP community (e.g. Leutbecher and Palmer 2008).

Uncertainty in the modelled atmospheric transport of CO₂ due to uncertain meteorological conditions can be quantified using ensemble forecasts with perturbed meteorological initial conditions according to the NWP analysis uncertainty (see Chen et al., 2019). An advantage of using ensembles is that they can capture the flow-dependent shape of the transport model errors. The spatial correlation structure in transport model errors has been ignored in most inversions using in situ observations but is likely important to consider especially when assimilating dense satellite XCO₂ observations to avoid potential biases.

Ensembles of different transport models can be used to quantify aspects of uncertainty in model dynamics and physics, for example by using different physics schemes (or, favourably, different models, i.e. multi-model) relating to turbulence, convection or diffusion. These ensembles represent uncertainty due to different model options; however, systematic errors inherent in the model or the multiple schemes remain unaccounted for in the derived uncertainty. An alternative method to estimate uncertainties in model physics is to use an ensemble of perturbed physical tendencies. Assuming the perturbations represent the uncertainty associated with the physics scheme, these ensembles can generate a suitable representation of model error. A recent study uses both an EDA and an ensemble of perturbed physical tendencies to quantify the model transport uncertainty for CO₂ modelling, which can be used to represent the model uncertainty in the CHE prototype (McNorton *et al.*, submitted). The uncertainty in biogenic fluxes related to the transport uncertainty is also highlighted and should be considered as part of the model uncertainty in any future CO₂ inversion system.

Numerical uncertainty in transport models arise from computational errors relating to discretization, interpolation and numerical diffusion. Accurate quantification of these errors is required for appropriate uncertainty attribution.

The representation error consists of two components. Firstly, the internal model component, which relates to the model inversion resolution being lower than that of the forward model (see Engelen *et al.*, 2002 for more details). Secondly, the error that arises from spatiotemporal differences between model and observations, for example a point measurement compared to a model grid box average. This error is expected to reduce as both forward and inverse model

resolution increases, and to an extent can be quantified using multi-resolution models (see Agustí-Panareda *et al.*, 2019 for more details).

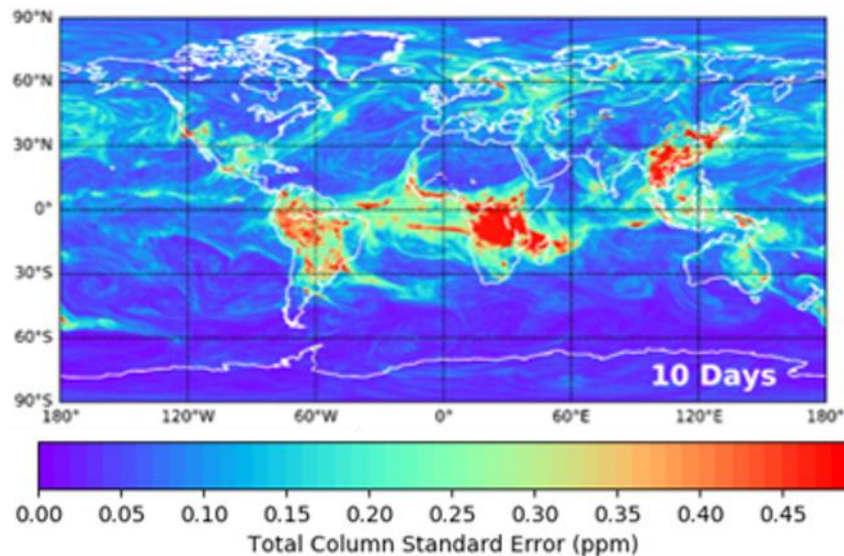


Figure 3: Global standard error of IFS model XCO₂ (ppm) across 50-member ensemble after 10 days. Errors shown are from model transport uncertainty relating to initial meteorological conditions and model physics.

A noteworthy aspect of the transport model error is that it saturates over time, and thus has consequences for the assimilation time window such that longer time windows will not suffer from increased transport model errors (long-time windows are preferable for the CO₂ problem because of the integrating capacity of the atmosphere). However, it should be noted that model bias does continue to grow with time.

3.4 Examples of posterior error quantification from OSSEs and QND studies

3.4.1 Observation Simulation System Experiments with an atmospheric transport inversion system

This example relies on an analytical Bayesian inversion system designed within CHE around the regional chemistry transport model CHIMERE (Menut *et al.*, 2013). The transport modelling domain covers the Western part of Europe with a horizontal resolution that varies between 50 and 2 km. The 2 km × 2 km-resolution zoom covers Northern France, a large part of Benelux and Western Germany. The analytical Bayesian inversion (Wu *et al.*, 2016) allows for the computation of the posterior uncertainty in the inverted flux budgets (its covariance matrix **A**) as a function of the observation operator **H** (connecting the fluxes to the observation vector, and mainly built on the transport model), the covariance matrices of the prior uncertainties **B** and the model and observation errors **R** following Tarantola (2005): $\mathbf{A} = [\mathbf{B}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}]^{-1}$. Actual observation values are not needed.

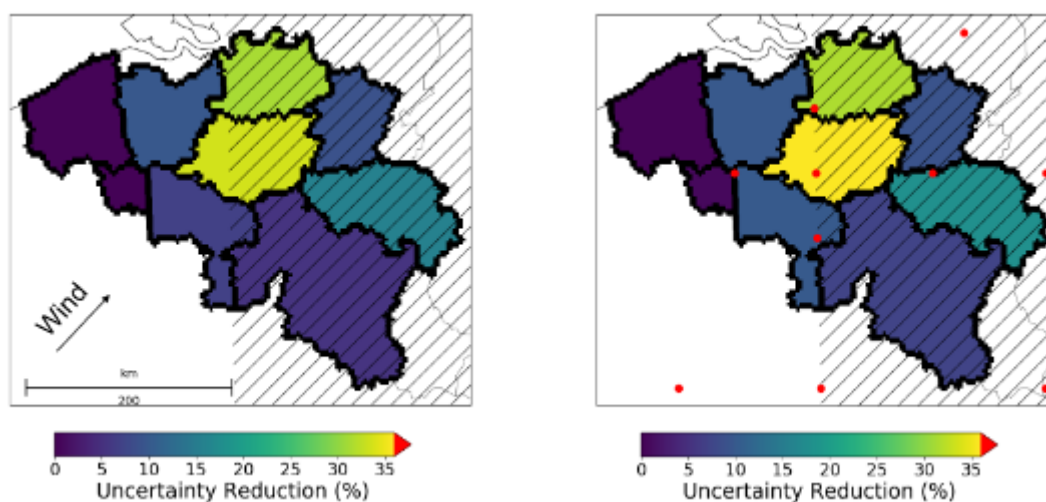


Figure 4: Uncertainty reduction for the fossil fuel CO₂ fluxes between midnight and 1 pm on 5 January 2015. Assimilated data are either (left) a CO₂ column image at noon (swath 200 km; σ = 1 ppm; hashed area) or (right) the same with surface CO in situ measurements (from 10 am to 4 pm; σ = 5 ppb; red dots).

Figure 4 shows an uncertainty reduction estimate for 1 day in January. Control variables in the estimation problem are biogenic CO₂ hourly fluxes and CO₂ and CO emissions from fossil fuel and biofuel in 6 anthropogenic sectors and ten regions (including one for the rest of the domain). The 1- σ prior uncertainty is set to 50% for the regional, city or point source hourly budgets of natural or anthropogenic fluxes from ecosystem models and inventories. Temporal auto-correlation of this prior uncertainty have a 3-hour temporal scale. No correlation is assumed between different regions/cities/point sources, sectors and between natural and anthropogenic emissions, but a correlation of 0.8 between anthropogenic CO₂ and CO prior emission uncertainties is assigned. The figure presents two configurations using or not CO surface measurements in addition to the satellite retrievals: a modest impact of the CO ground-based measurements on the estimated CO₂ flux is seen for that study day.

3.4.2 Quantitative Network Design with a Carbon Cycle Fossil Fuel Data Assimilation System

Quantitative Network Design (QND) is a technique that assesses the value of observations for constraining model uncertainties by propagating uncertainties through a modelling chain. The observations can be from a real or hypothetical network; thus, QND is useful for network design and to efficiently evaluate different observational strategies. Here the modelling chain is the Carbon Cycle Fossil Fuel Data Assimilation System (CCFFDAS), which is a global system that couples the Fossil Fuel Data Assimilation System (Asefi-Najafabady *et al.*, 2014) and the Carbon Cycle Data Assimilation System (Kaminski *et al.*, 2017).

CCFFDAS consists of two process-based models that simulate the fossil fuel emissions and terrestrial carbon cycle. The CO₂ fluxes from these models depend on a set of uncertain model parameters, which can be constrained by assimilating various observational data streams. The link between model parameters and observations are established through the process models and different forward models as described in Kaminski *et al.* (2019).

CO₂ surface fluxes from the fossil fuel and terrestrial biosphere models are linked to atmospheric CO₂ concentrations through the global atmospheric transport model TM3. The atmospheric transport is represented by pre-computed response functions. For the initial experiments over one week, the response functions provide the sensitivity of CO₂

concentrations to CO₂ fluxes within the same week. The atmospheric CO₂ concentration can then be sampled using different sampling strategies to correspond to e.g. in situ CO₂ or satellite XCO₂ observations.

The fossil fuel emissions model parameters are constrained by additional data streams including nightlight intensity and national total emissions from inventories for the two sectors. Nightlight observations are used as proxies for GDP and population density. Emission inventory data from e.g. IEA are treated as observations and can be assimilated to provide additional constraints on the process parameters in the fossil fuel emissions component.

The coverage and uncertainty (random and systematic) of XCO₂ observations are shown in Figure 5. This space-borne observation network is compared with a network of in situ observations with 15 and 141 sites. Nightlights are used as an additional data stream in all experiments, while national inventory data were left unassimilated except for in one experiment. After obtaining the posterior parameter uncertainties, the uncertainties were propagated forward through the modelling chain to provide uncertainties for national fossil fuel emissions from the two sectors for five selected countries.

Error! Reference source not found. lists the posterior fossil fuel emissions uncertainties for five different experiments. Assimilation of CO₂ observations and nightlights yield only marginal uncertainty reductions for the electricity generation sector, but for the other sector there is a noticeable difference in posterior uncertainties between assimilating in situ observations and XCO₂ from satellites: posterior uncertainties when assimilating XCO₂ from a single satellite are generally an order of magnitude smaller compared with when assimilating in situ CO₂ observations. Finally, simultaneous assimilation of XCO₂ observations and information from a national inventory results in another order of magnitude reduction in posterior uncertainties.

Table 2: Posterior uncertainty in national CO₂ fossil fuel emissions (MtC/week) during the first week of June 2008 for two sectors and five selected countries: Australia (AUS), Brazil (BRA), China (CHN), Germany (DEU), and Poland (POL).

Experiment	Other sector					Electricity generation sector				
	AUS	BRA	CHN	DEU	POL	AUS	BRA	CHN	DEU	POL
In situ 15 sites	9.03	16.70	177.31	12.18	4.70	0.28	0.17	2.36	0.43	0.23
In situ 141 sites	4.57	8.21	8.29	2.60	2.10	0.28	0.17	2.36	0.43	0.23
1 satellite	0.30	0.42	3.43	0.97	0.38	0.27	0.17	2.21	0.43	0.23
4 satellites	0.25	0.29	2.38	0.79	0.33	0.26	0.17	2.07	0.43	0.23
1 satellite and national inventory	0.03	0.03	1.84	0.08	0.05	0.04	0.06	0.07	0.07	0.05

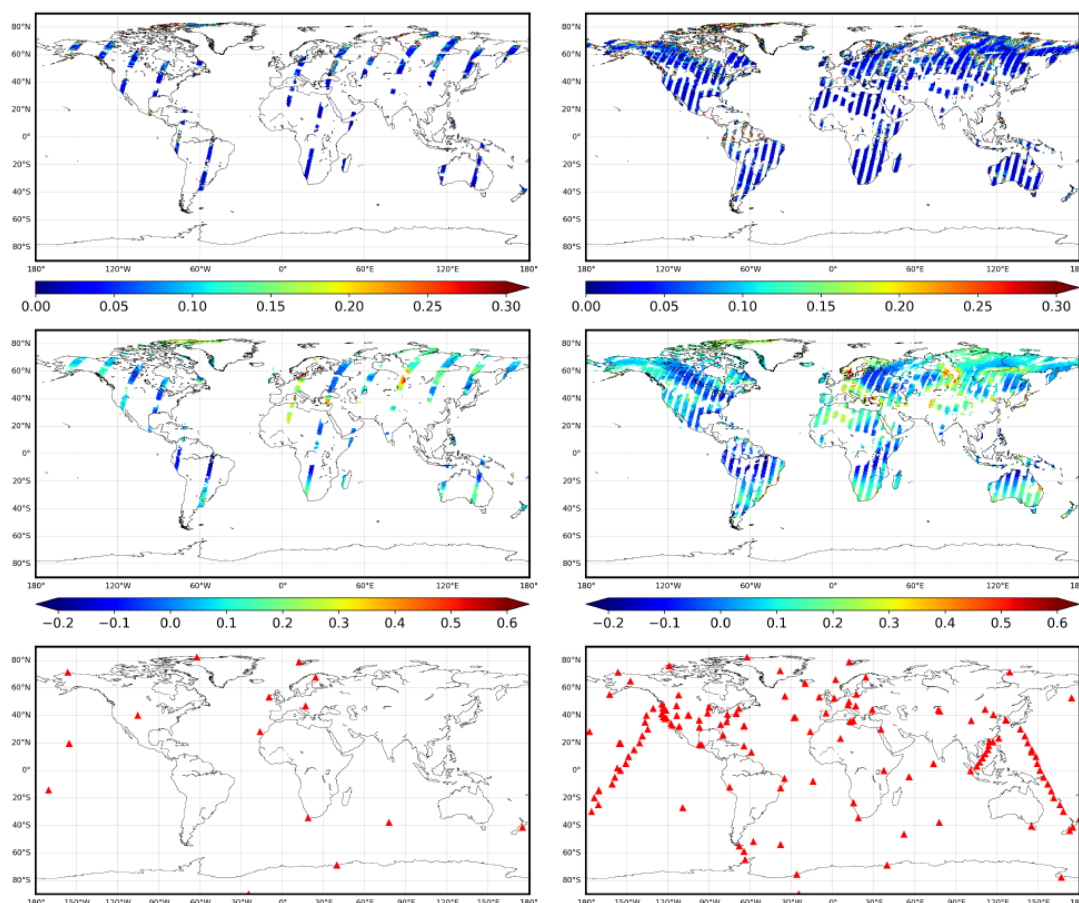


Figure 5: Upper four panels: Random (top) and systematic (middle) errors in CO₂ retrievals (ppm) from one (left) and four (right) satellites during the first day of June 2008. Bottom panels: Locations of in situ sites for network with 15 (left) and 141 (right) sites. Note that the retrieval errors shown here are aggregated on a 0.5° grid (individual 2 km by 2 km pixels have larger errors).

The QND approach provides not only posterior uncertainties (variances), but also the posterior covariances between process parameters. These covariances can indicate whether the observations are sufficient to separate between e.g. fossil fuel emissions from different countries or sectors.

The derived posterior uncertainty in an ensemble-based system must be robust and not suffer from undersampling failing to correctly represent the PDF. This has been illustrated with CCFFDAS by comparing the posterior uncertainty for the other sector calculated by inverting the full Jacobian with inverting an approximation of the Jacobian using the leading Eigenvalues from an Eigenvector decomposition of the full Jacobian. As can be seen in Figure 6 for the example countries Brasil and China the estimated posterior uncertainty using the first 20 Eigenvalues is substantially higher than from the full Jacobian: >800 MtC/yr versus 16 MtC/yr for Brasil, and >1100 MtC/yr versus 133 MtC/yr for China.

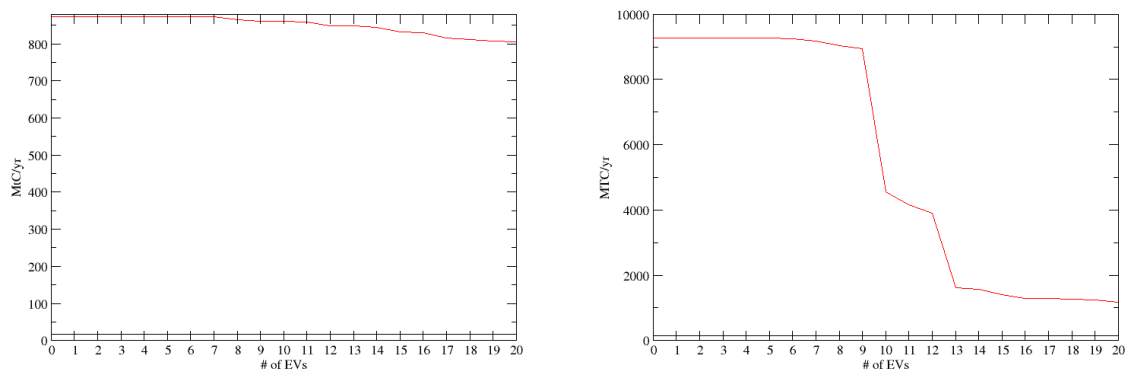


Figure 6: CCFFDAS posterior uncertainties of national total emissions (other sector and first week of June) from full Jacobian (black) and leading Eigenvalue approximation (red); left for Brazil and right for China.

At high resolutions (local, plume scale), the derivation of posterior estimates and representation of posterior uncertainty may be affected by highly nonlinear and non-Gaussian errors (e.g. representation error), which could pose problems for the assimilation scheme (e.g. consider a misaligned CO₂ plume).

3.5 Validation of posterior fluxes

For a full evaluation of the monitoring system, the posterior estimates need be evaluated against independent information as far as possible. Such evaluation or benchmarking activities are useful to demonstrate the quality of the development building blocks and the prototype system over time. An example for an existing benchmarking system for terrestrial biosphere models is the International Land Model Benchmarking project (ILAMP, Hoffman et al., 2016). A first approach for benchmarking atmospheric transport models has been outlined by Chevallier et al. (2019), however, focussing only on atmospheric CO₂ data. The atmospheric data should encompass multiple observation/variable types, e.g. flux-towers, surface concentrations, column concentrations and aircraft profiles. For the monitoring system this benchmarking needs to be more comprehensive and must evaluate the posterior results of the prototype. For this, it is important to establish independent observations, which are suitable for validation of posterior estimates and uncertainties at all temporal and spatial scales, for which posterior information is provided. Work for this has already begun within WP1 (in collaboration with the Global Carbon Project). It may be beneficial to consider three groups of observations for the evaluation: (1) Case studies, which can provide targeted information and potentially more observations than what is usually available; (2) Continuous observations to continually verify the performance of the operational system and detect drifts and biases; and (3) Observations (e.g. from remote sensing) that could be useful for validating the spatiotemporal variability or trends in the posterior estimates.

Validation exercises should consider uncertainties in the observations which are usually not accounted for, for example when validating posterior flux estimates over an urban environment, it might be suitable to use multiple flux sites over one gridbox if possible, to account for the representation error.

Since the available observations to evaluate the monitoring system are limited, cross checks against other systems (i.e. intercomparisons) and consistency checks within the system are necessary. Cross checks against other systems require the availability of inversion / data assimilation systems capable of yielding similar posterior fossil CO₂ estimates with uncertainties. These systems do not necessarily need to have the same complexity but should ideally span a range of approaches. In addition, such 'lighter' systems can also be used then

to estimate the potential posterior error reduction for different observational networks through the above mentioned (Sections 3.4.1 and 3.4.2) OSSE's and QND studies. Consistency checks need to be performed to ensure that the monitoring system correctly represent the underlying assumptions; these can also be done by OSSE's or identical-twin experiments.

4 Recommendations for the Operational CHE Prototype

This section provides recommendations for the configuration of the building blocks with respect to the uncertainty aspect to be implemented in the near-term future, i.e. in the next 3 to 5 years. Additional immediate development aspects of uncertainty representation for some of the individual building blocks, for instance observation uncertainty, methodological uncertainty, transport model uncertainty, are detailed in their specific reports. Here we mention some development aspects pertaining to the uncertainty representation in these building blocks.

The recommendations are listed in Table 3 with an indication of the temporal (NRT/reanalysis) and spatial (global/regional/plumes) scales.

4.1 Prior Information

For the prior uncertainty specification within the prototype, there are two general considerations:

- Both direct flux estimation by inversions and process model optimisation by data assimilation (or a combination of both), require information from the most fundamental level. As an example, derived uncertainties from transporting fluxes, require knowledge of uncertainties of the proxy data which informed the flux dataset. As a result, the representation of prior uncertainties within the monitoring system should start at the earliest possible stage of the compilation of a prior flux or parameter.
- Each directly actionable aspect of prior uncertainty needs to be incorporated into the development of the monitoring system at all scales (global/regional/local). This includes prior flux uncertainty, transport uncertainty and observation uncertainty.

4.2 Methodological Aspects

From a methodological aspect, it is important to adopt a consistent method (at all domains and streams) for the derivation of the posterior uncertainty. If, for any reason this will not be the case, then each individual method needs to be benchmarked to ensure consistency across scales and systems.

Future work also needs to address the potential of additional data streams (such as co-emitted species or radiocarbon) in reducing the posterior uncertainty. This should be done for direct transport inversions but also for data assimilation systems such as CCFFDAS. Some preliminary work on the potential of adding radiocarbon in CCFFDAS has already been performed assuming radiocarbon to be a perfect tracer of fossil fuel emissions. In such a case, radiocarbon could provide additional valuable information compared with using CO₂ observations alone. Additionally, it is desirable to extend the sectorialisation in FFDAS to resolve the 7 emission groups mentioned in Section 3.2. This could be done by implementing the model behind the emissions calculation for the 7 groups in the CCFFDAS, and thus more observations (such as traffic counts and other activity data) could be assimilated to further constrain posterior emission estimates and reduce the posterior uncertainty.

When considering ensembles as a representation of prior uncertainty, whether for transport or representation error, research should be performed into the trade-off between increasing

ensemble size or resolution, as both come at extra computational cost. Unlike resolution increase, ensemble size increase can be performed in parallel, potentially increasing energy costs but reducing wall time.

In terms of the inversion/data assimilation methodology underlying the CO₂ monitoring system, research needs to be performed addressing the question of adequately representing posterior uncertainties by the chosen method. When evaluating fossil CO₂ emission reduction measures the monitoring system needs to be capable of yielding not only estimates of these emissions but also of their uncertainties to be able to make robust statements on the reduction measures. This is particularly important for ensemble approaches. A PDF of the uncertainty at all scales can be represented using ensemble trajectories. But for this the ensemble size is important because undersampling fails to correctly represent the PDF and eventually introduces a new uncertainty.

4.3 Evaluation of posterior estimates and their uncertainty

As part of the quality control of the overall system each individual modelling building block as well as the posterior estimates need to be evaluated. In this respect, a powerful tool to assess the consistency of the posterior estimates and their uncertainties from atmospheric inversions are intercomparison studies as has been demonstrated in the past by the TRANSCOM project (e.g. Gurney et al., 2002) for the global scale and more recently by the EUROCOM project for the regional (European) scale (Monteil et al., 2019). Such intercomparison studies provide useful insights on the range of plausible posterior estimates as derived from the whole modelling chain and, as such, should be extended to cover also fossil CO₂ estimation.

Besides intercomparisons it is important to develop benchmarking metrics to a) evaluate the posterior uncertainty estimates as far as possible against independent observations and b) to demonstrate and document the fidelity of the CHE prototype. The development of these metrics need to go hand-in-hand with the creation of appropriate databases containing the required observations for the benchmarking (e.g urban eddy-covariance fluxes, direct activity data from different emissions sectors, citizen data such as traffic data collected by e.g. Google as far as these are not used in the assimilation).

Table 3: Immediate development needs of the prototype with respect to the uncertainty representation

Component	Domain	Stream	Recommendation	Estimated effort
Anthropogenic emissions uncertainty	global	NRT and reanalysis	Specify emission uncertainty for temporal profiles for different sectors at weekly, daily, hourly scales	12 months
			Uncertainty estimates on vertical profiles of emissions (e.g. Brunner et al. 2019)	12 months
	global, regional		Uncertainty estimates on modelled temporal profiles & spatial distributions with e.g. meteo predictors (residential heating) or traffic statistics (road sector) to support FFDAS approach.	12 months
			Evaluate uncertainty specification by consistency checks, i.e. cross check against other inventories	12 months
			Quantification of the range in emission ratios for co-emitted traces (CO and NO ₂) through literature studies (and in the longer term through dedicated field/lab experiments, see Section 5 and also D3.4)	6 months (literature review) 36 months (lab experiments)
	reanalysis		Sectorialisation of the fossil fuel emissions model and specification of prior uncertainties within individual sectors (e.g. error correlation in power generation sector within a country, road traffic error correlation in transport sector) and derive TL/AD of the respective observation operators for each sector	24 to 48 months (depending on the number of sectors)
Biogenic flux uncertainty	global, regional	NRT	Evaluate simplified models against independent data (e.g. flux data not used for model tuning)	6 months
			Quantify impact of uncertainty in mapping of land use on fluxes in global and regional models: classification, cover, including vegetation, urban and wetland mapping	12 months
	global, regional	reanalysis	Quantify range of land use change related emissions from DGVMs, simplified models, and statistical data-driven approaches	12 months

			Inter-comparison of DGVMs and simplified models and statistical data-driven approaches (multi-model ensemble to characterise uncertainty)	24 to 36 months
	Global, regional	NRT, reanalysis	Evaluate uncertainties in the observations of additional tracers to constrain biogenic fluxes (e.g. SIF, COS)	12 to 24 months
	global, regional	NRT, reanalysis	Evaluate uncertainties in the representation of additional tracers (SIF, COS) to constrain biogenic fluxes by process studies and comparison of observation operators with different complexity and derive TL/AD of the respective observation operators	24 to 36 months
Observation uncertainty	Global, regional, local	NRT, reanalysis	Develop and implement a validation strategy for CO ₂ M observations (XCO ₂ and NO ₂) following the approach outlined in Pinty et al. (2019).	36 months
			Develop and create quality-controlled databases with observations and their uncertainties for evaluation / benchmarking of the posterior estimates of the prototype: (1) targeted case studies (e.g. intensive urban flux monitoring campaigns), (2) continuous observations for continuously monitoring the system's performance, and (3) observations (e.g. from remote sensing) for validating spatiotemporal variability or trends.	12 to 18 months
	Global, regional		Extend and harmonise additional observations and their uncertainties for use in process model DA (urban eddy-covariance fluxes, nightlights, road traffic, census data (population density, GDP), inventories)	12 to 18 months
			Radiocarbon: terrestrial disequilibrium (see e.g. Miller et al., 2012; and Scholze et al., 2008 for ¹³ C), ocean exchange, nuclear power plants (Kuderer et al., 2018)	12 to 18 months
Inversion / data assimilation methodology	global, regional, local	NRT, reanalysis	Investigate the impact of larger ensemble size versus increased resolution in the representation of uncertainty by ensemble approaches	6 to 12 months

	global, regional	NRT, reanalysis	Adequate representation of posterior uncertainty on relevant spatio-temporal scales from methodological approach, for instance ensemble size, assimilation window length, model resolution (also of TL/AD)	12 months
			Quantification of the impact of approximations imposed by the various methodological approaches on the posterior uncertainty (definition of control vector, length of assimilation window)	24 months
	local	NRT, reanalysis	Fingerprinting CO ₂ plumes and investigating the impact of highly nonlinear and non-Gaussian error structures (e.g. representation error) on posterior estimates	6 to 12 months
Posterior evaluation / benchmarking	global, regional, local	NRT, reanalysis	Develop metrics to objectively evaluate/benchmark posterior estimates taking into account posterior uncertainty and uncertainty of the observations/data used for the evaluation	24 months
			Develop a framework for consistency checks (model intercomparisons)	24 months
	reanalysis	Support the availability of 'lighter' systems for cross checks (model intercomparison) of the posterior uncertainty estimate	12 to 36 months	

5 Research Priorities

Table 4: Research priorities linked to the domain (global, regional, local) and stream for application in the prototype: Near Real Time (NRT), or re-analysis (RA). An estimate of the effort required is given in person months.

Component	Domain	Stream	Recommendation	Estimated effort
Co-emitted species	Global, regional, local	NRT, RA	Research feasible co-emitters and uncertainty in their co-emission factors and emissions.	12-24 months
Process based flux models	Global, regional, local	NRT, RA	Develop anthropogenic emission models and quantify their uncertainty.	24 months
Process based flux models and benchmarking	Global, regional, local	NRT, RA	Investigate the feasibility of using (i.e. acquisition) citizen data (such as traffic counts or mobile network utilisation) for constraining sectorial activity	24 month
Constraining biogenic fluxes	Global, regional	RA	Investigate the uncertainties of observations constraining biogenic fluxes (SIF, COS) and their observation operators	12-24 months
Observations of radiocarbon	Global, regional, local	NRT, RA	Investigate measurement techniques for radiocarbon and their uncertainties.	24-36 months
Radiocarbon contamination	Global, regional, local	NRT, RA	Research uncertainties related to contamination of radiocarbon proxy by nuclear power plants and terrestrial disequilibrium.	12-24 months
Numerical uncertainty	Global, regional, local	NRT, RA	Investigate the numerical uncertainties within all models involved within the CHE prototype	36 months
Flux uncertainty estimates	Global, regional, local	NRT, RA	Improved inventories, e.g. NRT data and uncertainties for different sectors	24 months
Cross check methods	Global, regional, local	NRT, RA	maintain alternative (potentially lighter) approaches for cross checks	24 months

6 Conclusion

This progress report summarises the main building blocks in representing uncertainty in an integrated anthropogenic CO₂ emissions monitoring system. All components of this CHE Prototype are considered here to provide a consolidated view on the characterization of uncertainties. The individual components themselves are discussed in their respective (progress) reports: Observations in D5.1, emissions and transport models in D5.3, inversion /

data assimilation methodology in D5.5 and D5.9 provides a synthesis of these building blocks for an end-to-end prototype system. The focus of this report is first to list the uncertainty components of the individual building blocks for the prototype and how they contribute to the overall posterior uncertainty estimations, second to identify tools and metrics to evaluate and benchmark the posterior uncertainty estimates of the prototype, and third to identify the immediate development needs of the prototype with respect to the uncertainty representation as well as longer term research priorities together with an estimate of the required efforts. This progress report covers already all of the above mentioned aspects. For the final report we will re-assess the estimated efforts for the immediate development needs (here, they were only roughly approximated) and expand on the methodologies for benchmarking and evaluating the posterior uncertainty estimates of the prototype system. Furthermore, the report will be extended by discussing uncertainty analysis for establishing a set of requirements on the observation accuracy for reliable statements on CO₂ emissions trends to evaluate the impact of NDCs.

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D5.3. Agustí-Panareda, Anna (ECMWF) et al.; Progress report on service elements for CO₂ Emission and Transport Models Integration, 2019.

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