CO2 Human Emissions

Final report on service element requirements for uncertainty representation

Marko Scholze et al.

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D5.8 Final report on service element requirements for uncertainty representation

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1 Executive Summary

This deliverable document reports on the ingredients required for a robust representation of uncertainties in the main building blocks of the CHE prototype anthropogenic CO_2 emissions monitoring system including the prior, observation, model and methodological uncertainties. All components of this CHE prototype are considered here to provide a consolidated view on the characterisation of uncertainties. The individual components themselves are discussed in their respective reports: Observations in D5.2, emissions and transport models in D5.4, inversion / data assimilation methodology in D5.6 while 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 and prioritise the immediate development needs (to be achieved in the H2020 CoCO2 project) of the prototype with respect to the uncertainty representation as well as longer term research needs (potentially to be addressed in future Horizon Europe research calls) 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 system to correctly provide 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 needs beyond the near-term development needs (Table 4). Besides identifying the development needs this report also suggests a prioritisation of the near-term development steps for the prototype. The three most important and beneficial (in terms of posterior uncertainty representation) priorities are:

- uncertainty and bias reduction in biogenic flux estimation (by including additional observations, e.g. SIF),
- use of activity data (aircraft and ship movements, traffic density, energy use, etc.) for estimating/modelling fossil fuel emissions,
- benchmarking and evaluating the posterior uncertainty estimates of the prototype (including use of urban eddy covariance data, internal consistency checks and evaluation of ensemble spread in ensemble systems, e.g. using rank histograms, and intercomparisons between idealised setups).

The biogenic fluxes play an important role in the estimation of anthropogenic CO_2 emission from atmospheric concentration data because the atmosphere - with its integrating capacity - does not allow to distinguish between the sources of atmospheric CO_2. Hence, any improved knowledge on the biogenic fluxes, which are typically an order of magnitude larger than the anthropogenic emissions, will directly benefit to the quantification of anthropogenic CO_2 emissions. Knowledge on the biogenic fluxes can be improved by rigorous evaluation of terrestrial carbon cycle models against observations but also by model intercomparisons. Further, additional observations such as sun-induced fluorescence (SIF) can be used to constrain the photosynthesis process representation in the terrestrial carbon cycle models.

Activity data such as aircraft and ship movements, traffic density, energy use but also meteorological predictors (e.g. as a proxy for residential heating) contain important information for providing better and more timely estimates of fossil fuel emissions on high temporal and spatial resolution, and for reducing uncertainties in the prior estimates. Alternatively, these

data can also be used for constraining models of sectorial fossil fuel emissions that can be used as an integrated component in the prototype.

An evaluation and benchmarking system for posterior uncertainty estimates of the prototype could encompass two pillars. The first would include independent observations (e.g. eddy covariance data reported anthropogenic emissions) and would allow a comparison of the intrinsic uncertainty ranges provided by the prototype with the uncertainty ranges derived from independent observations. The second pillar could assess, for selected (and possibly idealised) cases, the impact of approximations imposed by the design of a prototype (e.g. the ensemble size) on its estimates of the intrinsic uncertainty. Such assessments would rely on alternative approaches allowing a more exhaustive representation of posterior uncertainty.

2 Introduction of the Building Block

2.1 Background

The CHE prototype aims at building a system to monitor the exchange of CO_2 and potentially other important man-made greenhouse gases like CH4 between the Earth's surface and the atmosphere with the use of observations (mostly in the atmosphere), models and prior information including the specification of uncertainties. The system is designed to support the Paris Agreement and follows the directive of the EC as described by the Task Forces on CO_2 (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 varying 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.

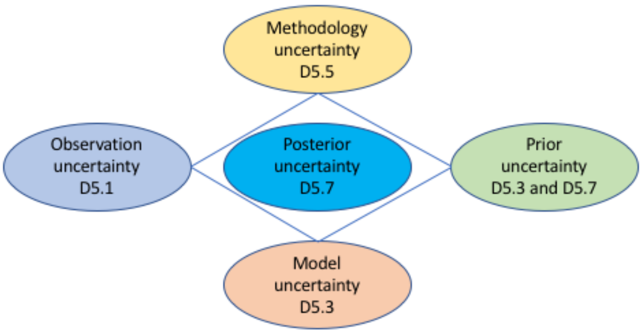

Figure 1: Building blocks of the CHE prototype with associated uncertainties and the specific deliverable reports associated with the specific building blocks.

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 CO_2 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 CO_2 monitoring system. This report outlines these aspects of uncertainty and expands on two methodologically 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 then 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 CO_2 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 CO_2 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 because 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 biogenic fluxes with uncertainties for use as prior information in the direct estimation of fossil fuel CO_2 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, which acts as the observation operator linking the emissions to the atmospheric concentrations, uncertainty in 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 and 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 numerical weather prediction (NWP) system for offline models.
- Structural uncertainty in the physics and parameterisation of model processes, including missing processes (e.g. atmospheric convection).

- 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, which 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 D5.2.

In short, the observation uncertainty consists of:

- Systematic and random error statistics of all observations.
- Model uncertainty including models to derive higher level products, e.g. retrieval algorithms to derive column CO_2 measurements from radiances).
- The representation error, which occurs because of coarse resolution model trajectories being compared to point measurements or finer resolution (e.g. satellite footprint) observations or mismatches 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.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverable

The objective of this deliverable is to report on requirements for representing the different sources of uncertainties in the localisation of CO_2 surface emission sources and the methods to reliably represent uncertainties and their variability with geographical, temporal and environmental conditions. Further, this report provides and prioritises recommendations for the development of a prototype MVS capacity as part of the H2020 CoCO2 project as well as recommendations for framing a future research agenda in support of an operational MVS capacity.

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.

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 *et al*. 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 estimates.	Choulga *et al*. 2020
Initial conditions (e.g. atmospheric 3D CO2 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 *et al.* 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 *et al*. 2020
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 *et al*. 2020
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 XCO2.	Connor *et al*. 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).	Agustí-Panareda *et al*. 2019
Methodological error	**Medium** - Considered in research. Accurate quantification requires further research.	Typically not considered so far.	Trudinger et al. 2007

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 that include:

- Deriving statistics of prior variables vs. observation comparisons
- Multi-model for the transport component (e.g. Offline chemical transport models 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 and planetary boundary layer schemes).
- 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 an evaluation of multiple aspects of posterior uncertainty and beyond just concentration data as currently done in atmospheric transport inversions, e.g. evaluation of the uncertainty in fluxes, parameters and any other proxy information.

As mentioned in Section 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 the EDGAR v4.3.2 dataset. Uncertainties are calculated dependent on the statistical development of a nation, with countries either being classified as having either 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, e.g. for aviation – Jet Kerosene, railways – Diesel, shipping – composition of 80% Diesel and 20% Residual Fuel Oil, and 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 ≥ 50%, then the methodology outlined by Frey (2003) is applied to ensure the lower probability density function (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 that the lower and upper uncertainty bounds are the 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.,* 2020). 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 or higher frequency).

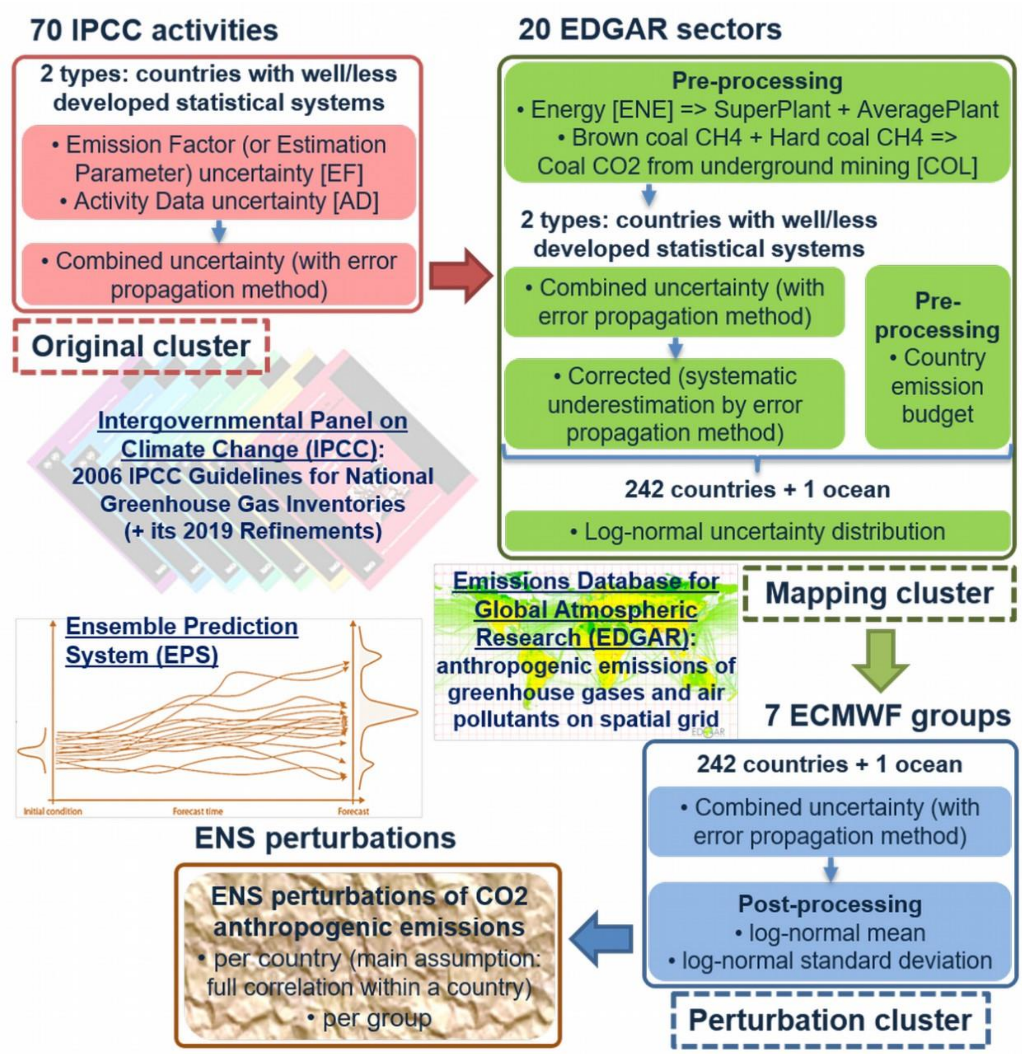

Figure 2: Schematic of methodology used to derive national annual and monthly uncertainties from activity and emission factor data through to a log-normal uncertainty distribution for 7 sectors per country.

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 CO_2 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 NWP, it is typically too computationally costly to calculate the full 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 CO_2 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 in the posterior.

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 CO_2 modelling, which can be used to represent the model uncertainty in the CHE prototype (McNorton *et al*., 2020). 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 CO_2 inversion system.

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

The representation error consists of two components. First, 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 be reduced 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).

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 CO_2 problem because of the integrating capacity of the atmosphere). However, it should be noted that model biases typically continue to grow with time.

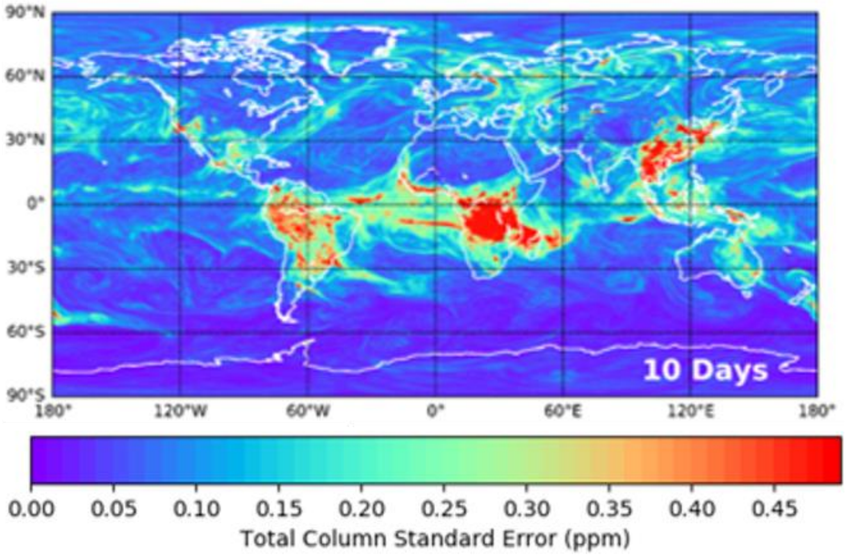

Figure 3: Global standard error of IFS model XCO2 (ppm) across 50-member ensemble after 10 days. Errors shown are from model transport uncertainty relating to initial meteorological conditions and model physics.

3.4 Examples of posterior error quantification from OSSE 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 shows an uncertainty reduction estimate for 1 day in January. Control variables in the estimation problem are biogenic CO_2 hourly fluxes and CO_2 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. The temporal auto-correlations 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 is assigned between anthropogenic CO_2 and CO prior emission uncertainties. Figure 4 presents two configurations using or not using CO surface measurements in addition to the satellite retrievals. A modest impact of the CO ground-based measurements on the estimated CO_2 flux is seen for that study day.

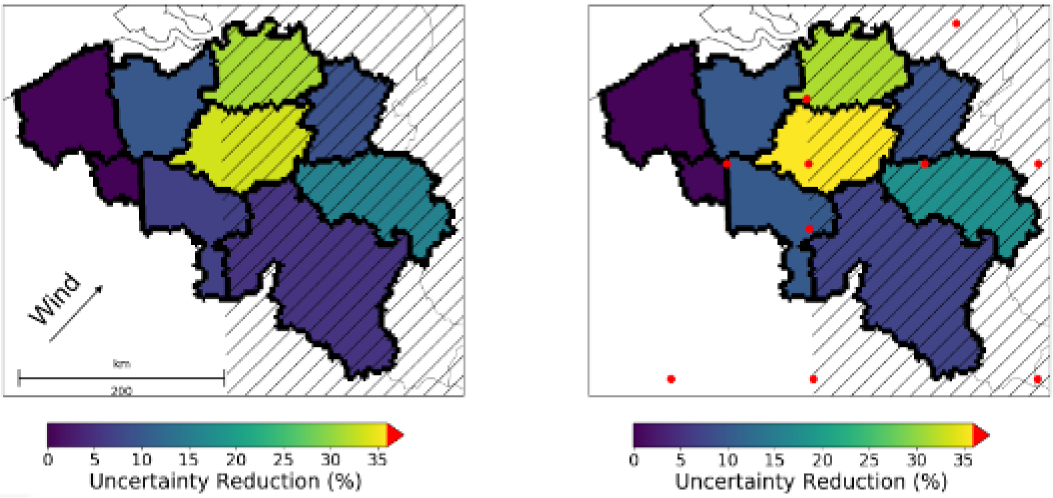

Figure 4: Uncertainty reduction for the fossil fuel CO2 fluxes between midnight and 1 pm on 5 January 2015. Assimilated data are either (left) a CO2 column image at noon (swath 200 km; σ = 1ppm; hashed area) or (right) the same with surface CO in situ measurements (from 10 am to 4 pm; σ = 5ppb; red dots).

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 CO_2 fluxes from these models depend on a set of uncertain model parameters, which can be constrained by assimilating various observational data streams. The links between model parameters and observations are established through the process models and different forward models as described in Kaminski et al. (2020).

CO_2 surface fluxes from the fossil fuel and terrestrial biosphere models are linked to atmospheric CO_2 concentrations through the global atmospheric transport model TM3. The atmospheric transport is represented by pre-computed response functions. For the experiments over one week, the response functions provide the sensitivity of CO_2 concentrations to CO_2 fluxes within the same week. The atmospheric CO_2 concentration can then be sampled using different sampling strategies that correspond to e.g. in situ CO_2 including radiocarbon or satellite XCO2 observations. Radiocarbon is a tracer that can be used to separate fossil fuel emissions (essentially radiocarbon-free) from natural carbon emissions (Levin et al., 2003).

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.

Table 2: Posterior uncertainty in national CO_2 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).

	Other sector					Electricity generation sector				
Experiment	**AUS**	**BRA**	**CHN**	**DEU**	**POL**	**AUS**	**BRA**	**CHN**	**DEU**	**POL**
In situ 15 sites	9.03	16.69	177.31	12.18	4.69	0.28	0.17	2.36	0.43	0.23
In situ 15 sites with radiocarbon	9.03	16.69	177.26	11.18	4.06	0.28	0.17	2.36	0.43	0.23
In situ 141 sites	6.84	11.85	10.75	3.76	3.12	0.28	0.17	2.36	0.43	0.23
In situ 141 sites with radiocarbon	5.71	8.75	9.09	2.99	2.31	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

The coverage and uncertainty (random and systematic) of XCO2 observations as well as the locations of the in situ stations are shown in Figure 5. This space-borne observation network is compared with a network of in situ observations with 15 and 141 sites of both only CO_2 and CO_2 and $^{14}CO_2$. 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 seven different experiments. Assimilation of CO_2 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 only in situ CO_2 observations. Also, adding radiocarbon observations has very little effect in the case of the 15-site network, however, for the larger 141-site network and countries with large terrestrial fluxes such as Brazil and Poland radiocarbon helps to separate fossil fuel emissions from natural exchange fluxes. Finally, simultaneous assimilation of XCO2 observations and information from a national inventory results in another order of magnitude reduction in posterior uncertainties.

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. Moreover, because the QND approach uses the full PDFs, it can be used to evaluate potential problems caused by undersampling in ensemble-based systems due to insufficient ensemble sizes. 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 Brazil 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 Brazil, and >1100 MtC/yr versus 133 MtC/yr for China. Thus, an ensemble with an insufficient ensemble size may not be able to take advantage of all information provided by observations without advanced ensemble techniques such as covariance localisation.

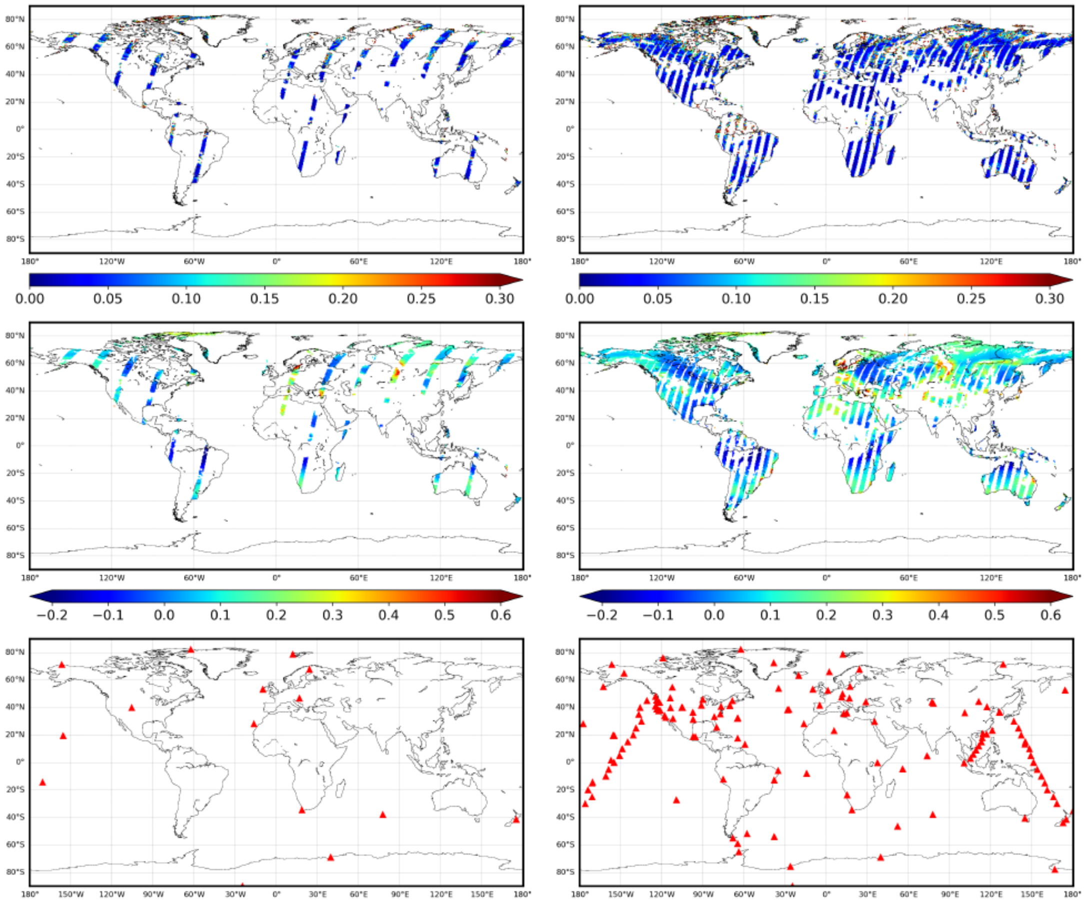

Figure 5: Upper four panels: Random (top) and systematic (middle) errors in CO_2 retrievals (ppm) from one (left) and four (right) satellites during the first day of June 2008. Bottom panels: Locations of in situ sites for network with 15 (left) and 141 (right) sites. Note that the retrieval errors shown here are aggregated on a 0.5° grid (individual 2 km by 2 km pixels have larger errors).

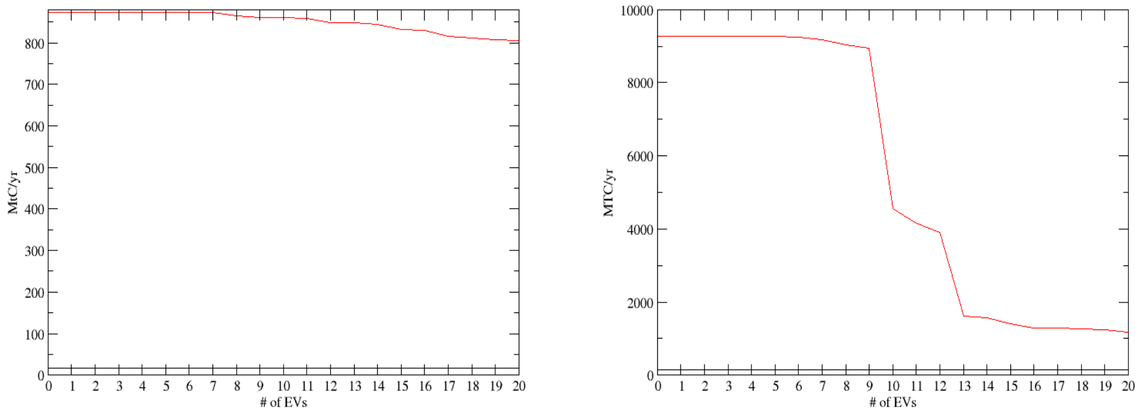

Figure 6: CCFFDAS posterior uncertainties of national total emissions (other sector and first week of June) from full Jacobian (black) and leading Eigenvalue approximation (red); left for Brazil and right for China.

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 CO_2 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 CO_2 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 on 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) Other 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 that 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 model grid box 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 CO_2 estimates with uncertainties. These systems do not necessarily need to have the same complexity but should ideally span a range of approaches. In addition, ‘lighter’ systems can also be used to estimate the potential posterior error reduction for different observational networks through the above mentioned (Sections 3.4.1 and 3.4.2) OSSE 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 OSSEs or identical-twin experiments.

4 Recommendations for the Operational CHE/CoCO2 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 (d5.2), methodological uncertainty (D5.6), transport model uncertainty (D5.4), 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 (near real time (NRT)/reanalysis) and spatial (global/regional/plumes) scales. These recommendations are prioritised by a colour coding according to their importance for the prototype to be developed in the H2020 CoCO2 project. Even a recommendation flagged as low priority is considered to be an important development step for the prototype within the near-term future.

In the next three subsections we provide some more general considerations on the representation and potential reduction of posterior uncertainties estimation.

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 prior 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 (as demonstrated in the OSSEs in Section 3.4.1) 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 CO_2 observations alone, especially for countries with large natural exchange fluxes (see Section 3.4.2). 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 on the trade-off between increasing ensemble size or model resolution, as both come at extra computational cost. Unlike resolution increases, it is more straightforward to take advantage of parallelisation to increase ensemble size, potentially increasing energy costs but reducing wall clock time.

In terms of the inversion / data assimilation methodology underlying the CO_2 monitoring system, research needs to be performed addressing the question of adequately representing posterior uncertainties by the chosen method. When evaluating fossil CO_2 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 effect of 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, as demonstrated in Section 4.2 even in the optimistic case of an ensemble spanned by the leading Eigenvectors.

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 CO_2 estimation. Intercomparisons should also be made with and within idealised setups, which allow to study methodological aspects such as the potential drastic overestimation of the posterior uncertainty in ensemble approaches as illustrated by Figure 5.

A useful metric to evaluate the reliability of ensemble systems are rank histograms (Candille and Talagrand, 2005) together with an estimate of the ensemble bias as proposed by Feng et al. (2019). Rank histrograms measure the spread of the ensemble by ranking the predicted variable according to the observations and assess the probability of occurrence of the observation within each histogram bin. A flat rank histogram in an unbiased ensemble indicates a reliable (consistent with observations) spread in the predicted variable.

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. The colour coding in the Recommendation cell refers to the priority for implementation of the recommendation in the prototype: red - high priority; yellow - medium priority; green - low priority. Note that even low priority recommendations are considered to be important development steps for the prototype within the near-term future.

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	6 months
			Uncertainty estimates on vertical profiles of emissions (e.g. Brunner et al. 2019)	6 months
	global, regional		Uncertainty estimates on modelled temporal profiles and spatial distributions with e.g. meteorological predictors (residential heating) or activity data such as traffic statistics (road sector) to support FFDAS approach.	12 months
			Evaluate uncertainty specification by consistency checks, e.g. 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 D3.4)	6 months (literature review) 24 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 tangent linear (TL) and adjoint (AD) models for the respective observation operators for each sector	< 24 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 dynamic global vegetation models (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)	18 months
	Global, regional	NRT, reanalysis	Evaluate uncertainties in the observations of additional tracers to constrain biogenic fluxes (e.g. SIF, COS)	18 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 and AD models for the respective observation operators	24 months
Observation uncertainty	Global, regional, local	NRT, reanalysis	Develop and implement a validation strategy for CO2M observations (XCO2 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) other observations (e.g. from remote sensing) for validating spatiotemporal variability or trends.	12 months
	Global, regional		Extend and harmonise additional observations and their uncertainties for use in process model data assimilation (urban eddy-covariance fluxes, nightlights, road traffic, census data (population density, GDP), inventories)	12 months
			Quantify uncertainty in radiocarbon observations due to: terrestrial disequilibrium (see e.g. Miller et al., 2012l; and Scholze et al., 2008 for ^{13}C), ocean exchange and nuclear power plants (Kuderer et al., 2018)	12 months

Inversion / data assimilation methodology	global, regional, local	NRT, reanalysis	Investigate the impact of larger ensemble size versus increased model resolution in the representation of uncertainty by ensemble approaches	6 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	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)	18 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 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)	18 months
		reanalysis	Support the availability of 'lighter' systems for cross checks (model intercomparison) of the posterior uncertainty estimate	24 months

5 Research Priorities

This section provides recommendations for further research needs in the building blocks with respect to the uncertainty aspect likely to be implemented through additional research activities within the Horizon Europe programme. Additional research needs for the uncertainty representation in some of the individual building blocks, for instance observation uncertainty (D5.2), methodological uncertainty (D5.6) and transport model uncertainty (D5.4), are detailed in their specific reports. The recommendations are listed in Table 4 with an indication of the temporal (NRT/reanalysis) and spatial (global/regional/plumes) scales. For these longer-term research recommendations no prioritisation is given.

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 into feasible co-emitters and uncertainty in their co-emission factors and emissions.	12 months
Process based fossil fuel models	Global, regional, local	NRT, RA	Develop anthropogenic emission models and quantify their uncertainty.	30 months
Process based fossil fuel 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 months
Constraining biogenic fluxes	Global, regional	RA	Investigate the uncertainties of observations constraining biogenic fluxes (SIF, COS) and their observation operators	12 months
Observations of radiocarbon	Global, regional, local	NRT, RA	Investigate measurement techniques for radiocarbon and their uncertainties	30 months
Radiocarbon contamination	Global, regional, local	NRT, RA	Research uncertainties related to contamination of radiocarbon proxy by nuclear power plants and terrestrial disequilibrium	18 months
Numerical uncertainty	Global, regional, local	NRT, RA	Investigate the numerical uncertainties within all models involved within the CHE/CoCO2 prototype	24 months
Flux uncertainty estimates	Global, regional, local	NRT, RA	Improved inventories, e.g. NRT data and uncertainties for different sectors	18 months
Cross check methods	Global, regional, local	NRT, RA	Maintain alternative (potentially lighter) approaches for cross checks	30 months

6 Conclusion

This report summarises the main building blocks in representing uncertainty in an integrated anthropogenic CO_2 emissions monitoring system. All components of this CHE Prototype are considered here to provide a consolidated view on the characterisation of uncertainties. The individual components themselves are discussed in their respective reports: Observations in D5.2, Emissions and Transport Models in D5.4 and Inversion / Data Assimilation Methodology in D5.6 and finally 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 and prioritise the immediate development needs of the prototype with respect to the uncertainty representation as well as to list the longer term research priorities together with an estimate of the required efforts.

It is suggested to prioritise the following three aspects in the identified near-term development needs:

- Reduction of uncertainty and bias in biogenic flux estimation (by including additional observations, e.g. SIF).
- Use of activity data (aircraft and ship movements, traffic density, energy use, etc.) for estimating and modelling fossil fuel emissions.
- Benchmarking and evaluating the posterior uncertainty estimates of the prototype (including use of urban eddy covariance data, internal consistency checks and evaluation of ensemble spread in ensemble systems using e.g. rank histograms, and intercomparisons between idealised setups).

The biogenic fluxes play an important role in the estimation of anthropogenic CO_2 emission from atmospheric concentration data because the atmosphere - with its integrating capacity - does not allow to distinguish between the sources of atmospheric CO_2. Hence, any improved knowledge on the biogenic fluxes, which are typically an order of magnitude larger than the anthropogenic emissions) will directly benefit to the quantification of anthropogenic CO_2 emission. Knowledge on the biogenic fluxes can be improved by rigorous evaluation of terrestrial carbon cycle models against observations but also by model intercomparisons. Further, additional observations such as sun-induced fluorescence (SIF) can be used to constrain the photosynthesis process representation in the terrestrial carbon cycle models.

Activity data such as aircraft and ship movements, traffic density, energy use but also meteorological predictors (e.g. as a proxy for residential heating) contain important information for providing better and more timely estimates of fossil fuel emissions on high temporal and spatial resolution and for reducing uncertainties in the prior estimates. Alternatively, these data can also be used for constraining models of sectorial fossil fuel emissions that can used as an integrated component in the prototype.

An evaluation and benchmarking system for posterior uncertainty estimates of the prototype could encompass two pillars. The first would include independent observations (e.g. eddy covariance data reported anthropogenic emissions) and would allow a comparison of the intrinsic uncertainty ranges provided by the prototype with the uncertainty ranges derived from independent observations. The second pillar could assess, for selected (possibly idealised) cases, the impact of approximations imposed by the design of the prototype (e.g. the ensemble size) on its estimates of the intrinsic uncertainty. Such an assessment would rely on alternative approaches allowing for a more exhaustive representation of posterior uncertainty.

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