Progress in coordinating efforts on uncertainty trade-off for fossil fuel emissions

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Co-ordinated by ECMWF

CO2 Human Emissions

D3.1 Progress in characterizing uncertainty for fossil fuel emissions

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1 Executive Summary

This document reports on progress to date within WP3 'Coordinating efforts on uncertainty trade-off for fossil fuel emissions' of the CO_2 Human Emissions (CHE) project. The aim of WP3 is ultimately to evaluate and coordinate possible improvements in the quantification of fossil fuel CO_2 emission uncertainty estimates from enhanced space-borne and in-situ observations. To this end, this work package involves both bottom-up inventory compilers and top-down observation analysts and atmospheric modellers to assess uncertainties in anthropogenic emissions and biogenic CO_2 fluxes, estimate the flux error covariances, and establish an optimal inversion strategy based on observing system simulation experiments (OSSEs) and quantitative network design (QND). All tasks within this WP have considerably progressed according to their work description in the Grant Agreement and no deviations from this work description have been identified. In Task 3.1, a dataset of global biogenic fluxes (gross primary production and net ecosystem exchange) have been derived for the period 2008-2017 and delivered to ECMWF. Task 3.2 has summarized the IPCC guidelines for CO_2 emission uncertainties and has compiled a table of the uncertainties on a per sector and per country basis. Task 3.3 has created a test dataset for tropospheric NO_2 column data from TROPOMI and is developing an inverse algorithm to derive TROPOMI-based NO_2 emission estimates. Task 3.4 has prepared an inversion system for OSSE studies, which currently assimilates synthetic in-situ and space-borne CO_2 observations. Finally, Task 3.5 has started configuring towards a coupled carbon cycle and fossil fuel data assimilation system for QND experiments to explore the benefit of different observations for monitoring and constraining fossil fuel emissions.

2 Introduction

2.1 Background

The CO_2 Human Emissions (CHE) project has been tasked by the European Commission to prepare the development of a European capacity to monitor anthropogenic CO_2 emissions. The monitoring of fossil fuel CO_2 emissions has to come with a sufficiently low uncertainty in order to be useful for policymakers. In this context, the main approaches to estimate fossil fuel emissions, apart from bottom-up inventories, are based on inverse transport modelling either on its own or within a coupled carbon cycle fossil fuel data assimilation system. Both approaches make use of atmospheric CO_2 and other tracers (e.g., CO and NOx) and rely on the availability of prior fossil fuel CO_2 emission estimates and uncertainties (as well as biogenic fluxes for the transport inverse modelling).

Observation-based CO and NOx emissions originate to a large extent from fossil fuel combustion and therefore can fingerprint fossil CO_2 sources. Relevant uncertainties in emissions are not limited to CO_2 but also include the additional tracers (CO, NOx), thereby creating substantial uncertainty in the ratios of CO_2 to other species both in time and space. Better uncertainty quantification of the tracers is aimed for with enhanced knowledge of the space infrastructure (Task 3.2).

WP3 evaluates the current status and possible improvements from enhanced space-borne and in-situ observation scenarios for fossil CO_2 emissions quantification based on observing system simulation experiments (OSSEs) and quantitative network design (QND) studies using different approaches (high resolution inverse transport modelling of CO_2 and co-emitted species (Task 3.4), advanced carbon cycle-fossil fuel data assimilation systems integrating atmospheric, terrestrial and socioeconomic datasets (Task 3.5)). For the inverse modelling and data assimilation systems, prior anthropogenic emissions and their uncertainties are needed (Task 3.3). In addition, the transport model inversions also require high-resolution prior biogenic fluxes with quantified uncertainties (Task 3.1). Task 3.4 and Task 3.5 constitute two different methods for evaluating the expected uncertainty reductions in fossil fuel estimates from potential space-borne CO_2 measurements. Based on these experiments WP3 will report on a set of inversion strategies blending bottom-up and top-down approaches for estimating fossil CO_2 emissions. For a robust estimate of the uncertainty, information from different sources needs to be brought together.

This deliverable provides an overview of work performed so far in WP3. The first specific deliverables from the completion of tasks in WP3, reporting in detail on work performed and accomplishments made within the respective tasks, are due month 21 (6/19). In order to demonstrate progress in WP3 within the first reporting period, this deliverable D3.1 provides a snapshot on the work performed within each task of WP3 to date. In each of the five subsections of section 3 a summary of the work done so far within each task of WP3 is presented. Comprehensive work descriptions will be provided in subsequent deliverable as indicated in each of the subsections of section 3.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverable

The objective of this deliverable is to provide a summary of the work progress made in WP3 within the first reporting period (10/17-12/18).

2.2.2 Work performed in this deliverable

After consultation with the partners involved with tasks T3.1–T3.5, a summary of the progress within WP3 has been compiled.

2.2.3 Deviations and counter measures

Not applicable.

3 Progress on tasks within WP3

3.1 Estimate biogenic fluxes and associated uncertainties from independent observations (Task 3.1)

Data-driven estimates of hourly net ecosystem exchange (NEE) and gross primary productivity (GPP) have been derived using in-situ eddy-covariance measurements, machine learning techniques, space-borne measurements of land surface parameters, and hourly meteorological information from the ECMWF ERA5 reanalysis dataset. Remote sensing data are based on the Moderate Resolution Imaging Spectroradiometer (MODIS; Tramontana et al. 2016). The global carbon flux estimates are available at 0.5-degree spatial resolution for the period 2008-2017, which includes the example years 2008 and 2015 that were chosen for this WP3. Figure 1 shows an example of the annual sum of NEE for 2008. The NEE and GPP datasets have been delivered to ECMWF.

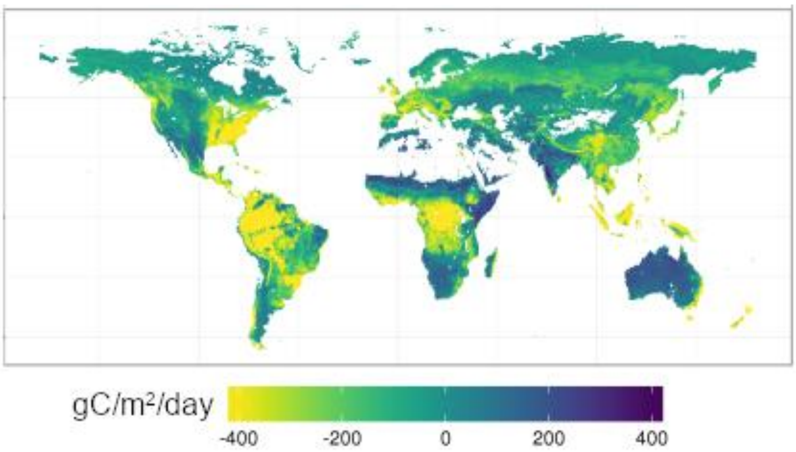

Figure 1: Example of global map showing the annual sum of net ecosystem exchange for 2008.

The data-driven NEE and GPP estimates rely on the methodology of FLUXCOM (Tramontana et al. 2016). Global NEE and GPP are derived through upscaling of eddy-covariance-derived net and gross carbon fluxes in the FLUXNET La Thuile dataset using the random forest machine learning algorithm. Compared with the FLUXCOM RS+meteo product (Tramontana et al. 2016), the biogenic flux dataset provided to the CHE project differs in the following ways: (1) only one machine-learning method (random forest) is used; (2) in addition to daily meteorological variables (same variables as in FLUXCOM RS+meteo), hourly meteorological variables are used as well as hourly potential radiation and its derivative; and (3) meteorology is based on ERA5, while FLUXCOM RS+meteo uses different meteorological reanalysis datasets. Compared with the prototype of data-driven sub-daily carbon flux estimates in Bodesheim et al. (2018), which is based on daily CRUNCEPv6 meteorology and half-hourly potential radiation and its derivative, this product uses daily ERA5 meteorology and additionally hourly data on air temperature, vapour-pressure deficit, and global radiation. Predictions are performed on an hourly basis instead of half-hourly.

First evaluations of the products have shown higher sub-daily variability, slight changes in the shape of the diurnal cycle in some regions of the Earth as well as a lower annual global land sink compared to the approach in Bodesheim et al. (2018).

A complete description of work performed in Task 3.1 and the results will be provided in the forthcoming deliverable report D3.2 due in month 21.

3.2 Provide emission uncertainties and correlations from inventories and statistics (Task 3.2)

The methodology to calculate CO_2 emission uncertainties based on IPCC guidelines has been finalised. Emission uncertainties are calculated for all world countries, under the assumption of two categories of world countries, depending on whether the country's statistical infrastructure is well or less developed. For well-developed statistical infrastructure, emission uncertainties are lower, while less developed statistical infrastructure countries have higher emission uncertainties. An ongoing sensitivity analysis is investigating the impact of the well or less developed infrastructure assumption for China, India, and Russia on the global emission uncertainty.

A table has been created that details the emission uncertainties on a per (sub)sector and per country-type basis. Six main sectors were identified for the CO_2 emissions to keep a reasonable 6x6 error covariance matrix. The per country and per sector-calculated uncertainties have been discussed in a meeting between JRC and ECMWF in Ispra on 18th-

19th September 2018 and the final product has been delivered to ECMWF. Analysis of the uncertainties is in progress.

A complete description of work performed in Task 3.2 and the results will be provided in the forthcoming deliverable report D3.3 due in month 21.

3.3 Explore the role of satellite observations of NOx for estimation of fossil CO_2 emissions (Task 3.3)

Top-down NOx emissions derived from both the Ozone Monitoring Instrument (OMI) and the Tropospheric Monitoring Instrument (TROPOMI) will be used to fingerprint CO_2 emissions on the same resolution by applying a ratio of emission factors of NOx and CO_2 based on the bottom-up emission inventories that are available within WP3 and the CHE project. These emission ratios, however, carry large uncertainties and should be used with caution. An inverse algorithm is currently being developed to derive NOx emissions from TROPOMI column-averaged NO_2 observations. The algorithm is based on an in-house developed algorithm called DECSO (Ding et al., 2017). Currently, OMI observations are used for the NOx emission estimates and emissions are derived on a 0.25-degree spatial resolution.

TROPOMI NO_2 retrievals have been analysed to determine how to take advantage of the higher spatial resolution and signal-to-noise ratio of this instrument compared with OMI. The NOx emissions from TROPOMI will be derived on a higher spatial resolution of 0.125 degrees, though for smaller regions than with OMI because of computational limitations. A typical size of the regions for TROPOMI-derived NOx emissions is 1000 km × 2000 km.

The first step toward TROPOMI-based NOx emission estimates is a refinement of the tropospheric NO_2 retrieval algorithm. TROPOMI tropospheric NO_2 column data are now operational and version 1.2 was recently made available. A tropospheric NO_2 column test dataset covering several months of 2018 is being reprocessed. The TROPOMI NO_2 algorithm is based on a DOAS retrieval for the slant column, in which the vertical stratospheric column is subtracted based on an NO_2 forecast from an assimilation system. An example of the tropospheric NO_2 retrieval of TROPOMI over Europe on 16 October 2018 is given in Figure 2. Clouds are shown with a white transparency depending on the cloud fraction. Figure 3 shows the monthly mean of tropospheric NO_2 for August 2018 based on TROPOMI observations.

A complete description of work performed in Task 3.3 and the results will be provided in the forthcoming deliverable report D3.4 due in month 27.

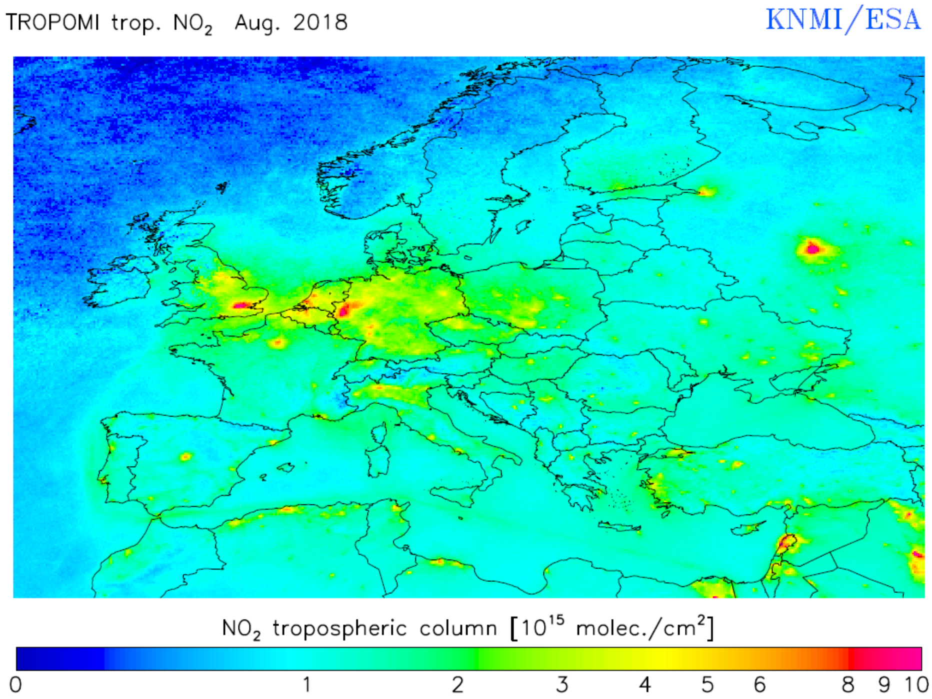

Figure 2: Tropospheric NO2 based on TROPOMI observations over Europe on 16 October 2016.

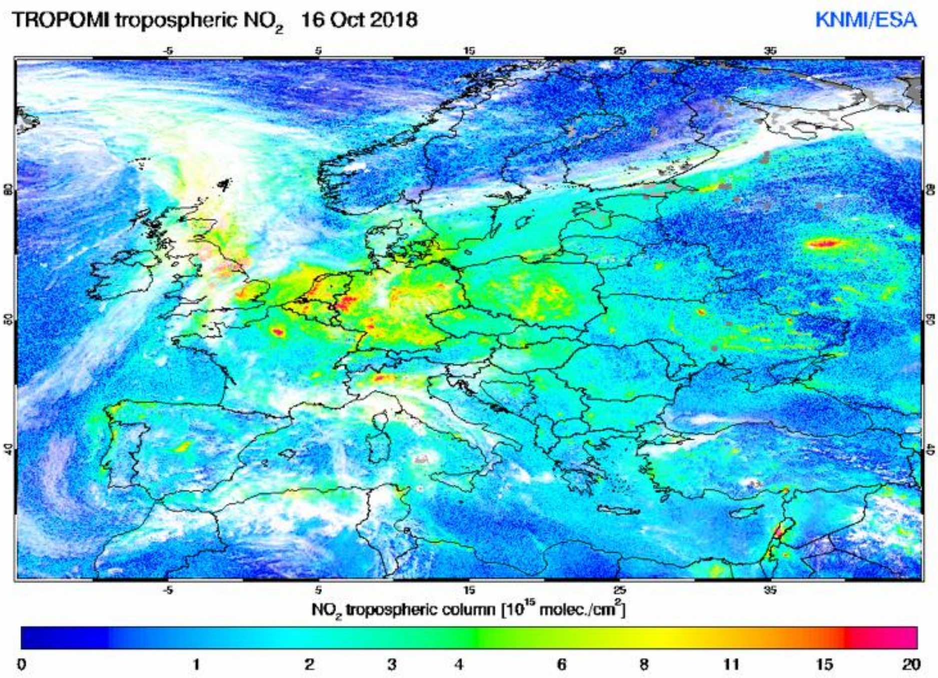

Figure 3: The monthly mean tropospheric NO2 based on TROPOMI observations for August 2018.

3.4 Conduct OSSEs with an inverse transport modelling system to establish inversion strategy (Task 3.4)

An inversion system has been prepared to assimilate space-borne and in-situ CO_2 and CO and in-situ radiocarbon observations. The inversion system is based on an analytical inversion framework (Wu et al., 2016) with a dedicated configuration of the CHIMERE transport model (Menut et al., 2013). The domain of this configuration 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, Benelux and Western Germany (Figure 4).

So far, the inversion system has only been implemented to constrain the CO_2 fluxes based on the assimilation of CO_2 data. It temporarily relies on anthropogenic emission maps that result from the merge of various products from the University of Stuttgart/IER (Vogel et al., 2010), until the dedicated products from partner TNO are available. Similarly, the inversion system currently relies on CO_2 land natural fluxes based on 8-km-resolution Vegetation Photosynthesis and Respiration Model (VPRM) simulations (Mahadevan et al., 2008, Kountouris et al., 2018), while the final system will use the 1-km-resolution VPRM simulations that will be generated by partner MPI-Jena.

A first inversion test has been conducted focusing on the inversion of CO_2 anthropogenic and biogenic fluxes in Belgium for 2 different days (on 3 February 2015 and 2 July 2016). The system controls hourly budgets (over 24 hours) of the anthropogenic and biogenic CO_2 fluxes for 9 administrative regions (Figure 5) and for one area covering the rest of the transport modelling domain.

Different scenarios of synthetic and (at this stage) highly theoretical CO_2 observation systems have been considered, with the inclusion of high-resolution CO_2 space-borne images for some of these scenarios (e.g. the hashed lines in Figure 6: theoretical satellite pass at 12h over Belgium) and different scenarios for the CO_2 in-situ continuous measurement networks. In-situ networks were derived from existing networks and theoretical coarse or dense potential extensions (e.g., the red points in Figure 6: theoretical coarse network). Following the traditional strategy of global to regional scale inverse modelling, the inversion system was assumed to assimilate hourly averages of the in-situ data during late morning and afternoon only (between 10h and 16h). Inversions usually assimilate data during the afternoon only (e.g., Kadygrov et al., 2015), but the assimilation window has been slightly extended here.

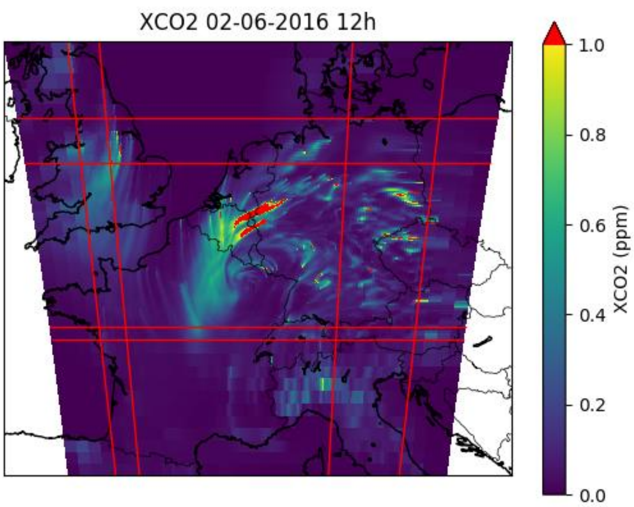

Figure 4: XCO_2 calculated from a CHIMERE simulation for 2 July 2016 at 12h. The red lines delimit the resolution changes (from 2 km to 10 km and then 50 km from the middle to the edges of the domain).

Figure 5: Correspondences between regions defined in this deliverable and the Belgian provinces.

The set of inversion statistical parameters in the OSSEs assumes a 1-sigma prior uncertainty of 50% in the regional hourly budgets of natural or anthropogenic fluxes from ecosystem models and inventories (a set up similar to that of Broquet et al., 2018). Temporal auto-correlation of this prior uncertainty with a 3-hour temporal scale is also accounted for but the correlation of the prior uncertainties between different regions (and between natural and anthropogenic emissions) is ignored. The errors associated with the observations and the transport model are presently accounted for in a simple way by setting the observation-and-model-error standard deviation to 5 ppm for the hourly in-situ data, to 1 ppm for the space-borne XCO_2 data, and ignoring temporal and spatial correlations in these errors and possible retrieval biases.

An analysis of the uncertainty reductions was performed for various budgets of anthropogenic and biogenic CO_2 fluxes, at the 1-hour to 24-hour scales (e.g., 02 July 2016, Figure 6) and at the regional to national scale. Furthermore, the problem of separability of the flux signal between anthropogenic and biogenic components was analysed for a given region (e.g., 02 July 2016, Figure 7), or between consecutive hours for the anthropogenic component, or between adjacent regions. First results showed uncertainty reductions between 0 and 20% for the majority of the regional budgets over 24 hours. Uncertainty reductions were higher for the morning budget because there are more observations than during the afternoon, and in particular satellite data at 12:00 mostly constrained the fluxes between 08:00 and 12:00. In the example given in Figure 6, the satellite pass decreased the uncertainty mainly for the regions within its field of view and these reductions reached 50% for the 24-hour budgets.

This inversion framework will serve as a core for the final atmospheric inversion system, built with new flux maps provided in the CHE project for year 2015 (TNO-CAMS81, 1/10° × 1/20°, 1 h and VPRM, 1 km × 1 km, 1 h). The same code will be used and the control vector will be extended to cities and administrative regions of the Northern France, Benelux and West Germany area and to larger regions outside this area. The first results for Belgium will drive this definition of the control vector over the whole West Europe area in a more precise and adapted way.

A complete description of work performed in Task 3.4 and the results will be provided in the forthcoming deliverable report D3.5 due in month 36.

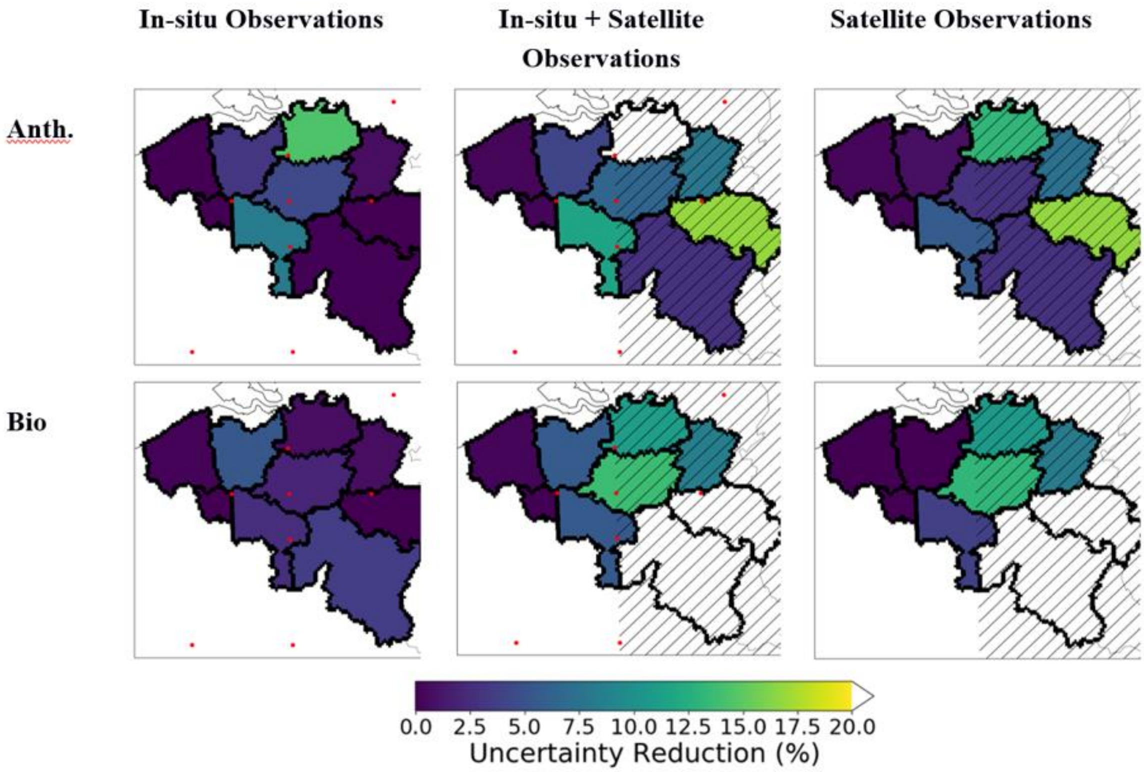

Figure 6: Uncertainty reductions between prior and posterior daily anthropogenic (top) and biogenic (bottom) regional budgets over 24 hours. Day 02/06/2016. With in-situ observations only (left; one per hour between 10h-16h, red points) and with a satellite pass (right; at 12h, hashed area). The satellite pass mainly decreases the uncertainty for the regions within its field of view and these reductions reach 50% for the biogenic emission budget of the Namur/Luxemburg region (south-eastern Belgium).

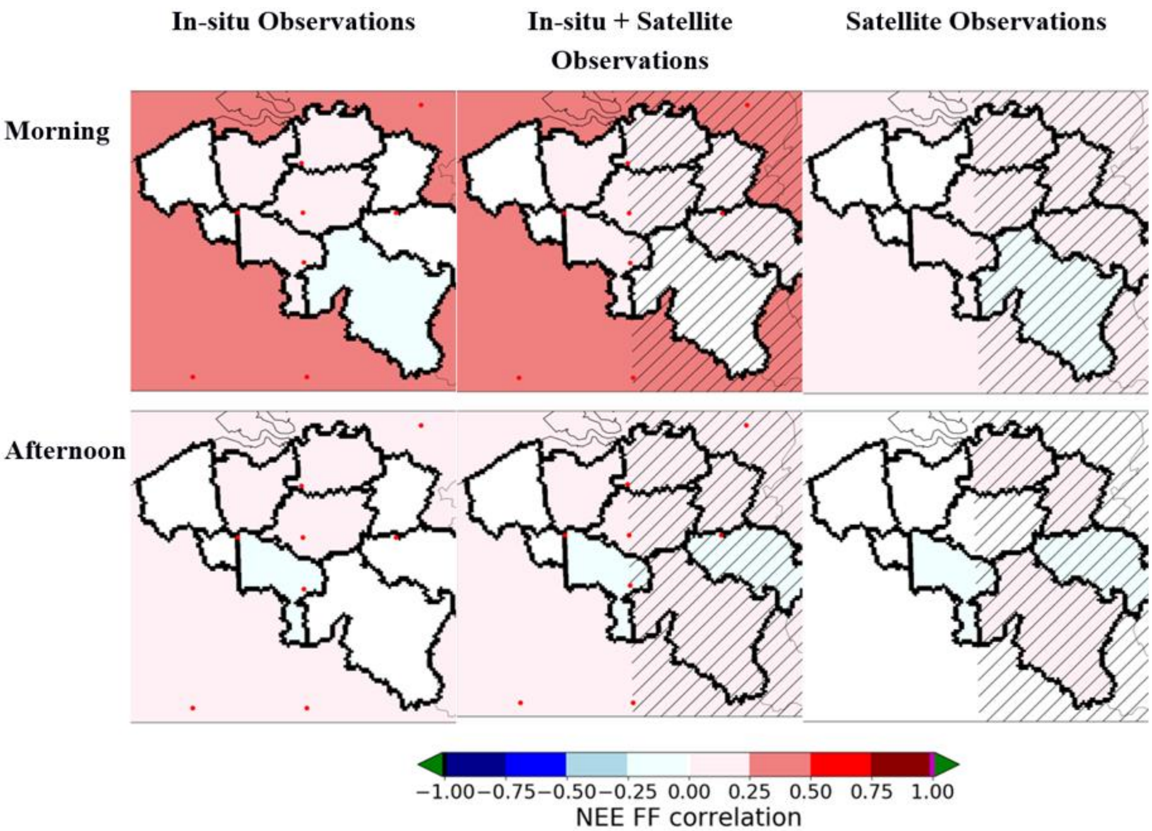

Figure 7: Correlations between posterior uncertainties in the anthropogenic and biogenic budgets, in the morning (top) and in the afternoon (bottom); negative values associated to relatively high posterior uncertainties are indicative of difficult separation between the different flux components (Broquet et al., 2018). Day 02/06/2016. With in-situ observations only (left; one per hour between 10h-16h, red points) and with a satellite pass (right; at 12h, hashed area).

3.5 Perform QND experiments with an advanced data assimilation system to establish inversion strategy (Task 3.5)

The Carbon Cycle Data Assimilation System (CCDAS; Kaminski et al. 2017) and Fossil Fuel Data Assimilation System (FFDAS; Asefi-Najafabady et al., 2014) are being configured for coupled CCFFDAS experiments in QND mode. The modelling framework for CCFFDAS is illustrated in Figure 8. Prior CO_2 fluxes and error covariances are provided by a fossil fuel emissions model and a terrestrial ecosystem model and linked to atmospheric CO_2 observations through the TM3 atmospheric transport model. CCDAS, FFDAS, and TM3 runs are ongoing.

The benefit of additional observations for constraining fossil fuel emissions will be quantified through the QND approach. QND performs a rigorous uncertainty propagation from the observations to a target quantity of interest relying on the indirect link from the observations to the target variables established by a numerical model, in this case CCFFDAS illustrated in Figure 8. Uncertainties in process parameters, external forcing/boundary values, and initial conditions are defined in a control vector (orange oval in Figure 8), which should cover all input quantities with high uncertainty and high impact on simulated observations and target quantities (Kaminski et al., 2012; Rayner et al., 2016). More information about the control vector for CCFFDAS is detailed below where the models are introduced.

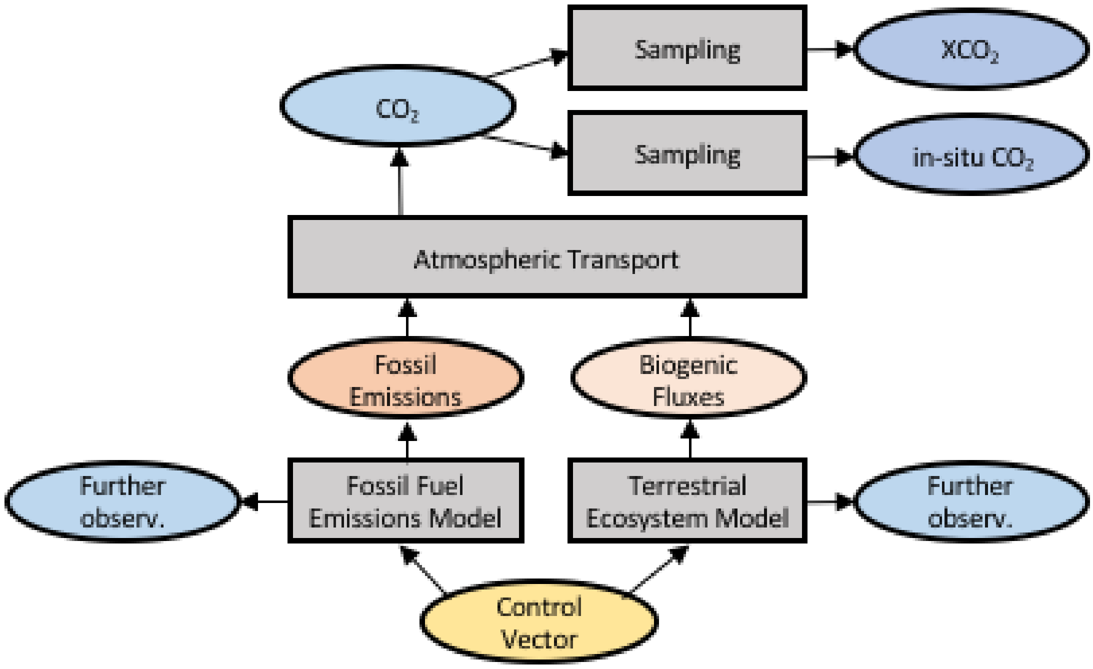

Figure 8: Modelling framework with information flow in CCFFDAS. Boxes represent calculation steps by models, blue ovals observables, orange oval control vector (model parameters and initial condition), and red ovals target quantities (fossil emissions, terrestrial fluxes).

The target quantity may be any quantity that can be extracted from a simulation with the underlying model, but also any component of the control vector. In the general case, where the target quantity is not part of the control vector, the QND procedure operates in two steps (Figure 9). The first step (inversion step) uses the observational information to reduce the uncertainty in the control vector, i.e. from a prior to a posterior state of information. The second step (prognostic step) propagates the posterior uncertainty forward to the simulated target quantity. For CCFFDAS, available target quantities are the 2008 national totals per sector and natural fluxes for selected countries over the globe. Further target quantities are sectorial emissions at individual grid cells (in megacities).

Another essential component of the data assimilation system is the observation operator, which translates model state information into observational variables. All observation operators have been implemented for CCFFDAS, which include national total fossil fuel CO_2 emissions provided by International Energy Agency, nightlights, column-averaged space-borne CO_2 observations, and in-situ CO_2 observations.

The underlying model for the fossil fuel CO_2 emissions is based on the Kaya identity (Nakicenovic, 2004) using a sectorial approach. Two sectors are defined for CCFFDAS: a power generation sector and all other emissions denoted as the “other” sector. For the fossil fuel emission model, the following process parameters are included in the control vector: per capita GDP (per gridcell), energy intensity (global value), carbon intensity (per country), nightlight scaling (global value), and power plant emissions from CARMA (per individual power plant).

The terrestrial biosphere model used to calculate the natural terrestrial biosphere CO_2 exchange fluxes is conceptually similar to the one used by Kaminski et al. (2002) and based on Knorr and Heimann (1995). The model operates on a 0.5 degree global grid and divides the global terrestrial biosphere into 8 land cover classes (or plant functional types) based on the MODIS land cover classification (Friedl et al., 2010). The CCFFDAS control vector includes two parameters per plant functional type for the terrestrial biosphere model, one controlling the light use efficiency, and the other one relating respiration to temperature.

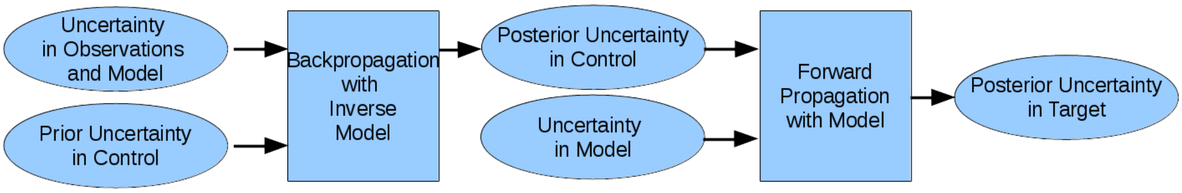

Figure 9: Data flow through two-step procedure of QND formalism. Oval boxes denote data, rectangular boxes denote processing. Figure taken from Kaminski and Rayner (2017).

A complete description of work performed in Task 3.5 and the results will be provided in the forthcoming deliverable report D3.6 due in month 36.

4 Conclusion

This document summarises the progress to date within the different tasks of WP3 ‘Coordinating efforts on uncertainty trade-off for fossil fuel emissions’ of the CHE project. All partners have made considerable progress towards the goals of WP3 within the first reporting period (10/17-12/18) and no deviations have been encountered. In Task 3.1, a dataset of global biogenic fluxes (GPP and NEE) have been derived for the period 2008-2017 and delivered to ECMWF. Task 3.2 has summarized the IPCC guidelines for CO_2 emission uncertainties and has compiled a table of the uncertainties on a per sector and per country-type basis. Task 3.3 has created a test dataset for tropospheric NO_2 column data from TROPOMI and is developing an inverse algorithm to derive TROPOMI-based NO_2 emission estimates that will be used to derive anthropogenic CO_2 emissions based on CO_2/NOx emission ratios. Task 3.4 has prepared an inversion system for OSSE studies, which currently assimilates synthetic in-situ and space-borne CO_2 observations. Task 3.5 has started configuring a coupled carbon cycle and fossil fuel data assimilation system for QND experiments to explore the benefit of different observations for constraining fossil fuel emissions.

This deliverable will serve as a reference document reporting on progress within the first reporting period (first 15 months) in WP3 of the CHE project.

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Document History

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0.2	Hans Chen Marko Scholze	07/12/2018	Taking into account comments from WP partners
1.0	Hans Chen Marko Scholze	20/12/2018	Taking into account comments from internal review

Internal Review History

Internal Reviewers	Date	Comments
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Eirini Boleti / Hugo Denier van der Gon (TNO)	13/12/2018	Approved with comments

Estimated Effort Contribution per Partner

Partner	Effort
ULUND	0.5 PM
Total	**0.5 PM**