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METHODS
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The CO_2 Human Emissions (CHE) Project: First Steps Towards a European Operational Capacity to Monitor Anthropogenic CO_2 Emissions

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The Paris Agreement of the United Nations Framework Convention on Climate Change is a binding international treaty signed by 196 nations to limit their greenhouse gas emissions through ever-reducing Nationally Determined Contributions and a system of 5-yearly Global Stocktakes in an Enhanced Transparency Framework. To support this process, the European Commission initiated the design and development of a new Copernicus service element that will use Earth observations mainly to monitor anthropogenic carbon dioxide (CO_2) emissions. The CO_2 Human Emissions (CHE) project has been successfully coordinating efforts of its 22 consortium partners, to advance the development of a European CO_2 monitoring and verification support (CO2MVS) capacity for anthropogenic CO_2 emissions. Several project achievements are presented and discussed here as examples. The CHE project has developed an enhanced capability to produce global, regional and local CO_2 simulations, with a focus on the representation of anthropogenic sources. The project has achieved advances towards a CO_2 global inversion capability at high resolution to connect atmospheric concentrations to surface emissions. CHE has also demonstrated the use of Earth observations (satellite and ground-based) as well as proxy data for human activity to constrain uncertainties and to enhance the timeliness of CO_2 monitoring. High-resolution global simulations (at 9 km) covering the whole of 2015 (labelled CHE nature runs) fed regional and local simulations over Europe (at 5 km and 1 km resolution) and supported the generation of synthetic satellite observations simulating the contribution of a future dedicated Copernicus CO_2 Monitoring Mission (CO2M).

Keywords: carbon dioxide monitoring, green house gas emission, earth system approach, paris agreement, global stocktake

INTRODUCTION

The CO_2 Human Emissions project (CHE, https://che-project.eu/) has responded to the task set by the European Commission to coordinate and support the development of a European capacity to monitor anthropogenic carbon dioxide (CO_2) emissions. Designed as a Coordination and Support Action, CHE has advanced on the building blocks of a CO_2 Monitoring and Verification Support (CO2MVS) for the Paris Agreement of the United Nations Framework Convention on Climate Change (UNFCCC). This historical binding pact signed by 196 nations in 2015, aims at limiting greenhouse gas emissions through Nationally Determined Contributions and a 5-yearly Global Stocktakes process that sit in an Enhanced Transparency Framework. To support this process the European Commission initiated the design and development of a new Copernicus service element that will use Earth observations (EOs) to mainly target anthropogenic CO_2 emissions. This is a major observational, technological, infrastructural and scientific challenge. The monitoring of fossil fuel CO_2 emissions must come with a reported uncertainty estimate that can be useful for policymakers (e.g., for targeting actions to lower uncertainties in hotspots of interest). In this context, the main approaches to estimate fossil fuel emissions, apart from the inventories, are based on the Earth observations and modelling. Inverse transport models, either used on their own or within a coupled carbon cycle fossil fuel data assimilation system, provide these so called "top-down" emission estimates. These can be driven by observations of not only CO_2 but also co-emitted species such as nitrogen oxides (NO_x) and of variables that constrain the emission processes such as nightlight intensity, used to locate human activity related to anthropogenic CO_2 emissions, or Fraction of Absorbed Photosynthetically Active Radiation (FAPAR), used to constrain the biogenic CO_2 naturally absorbed by vegetation during the photosynthesis.

The setting up of a CO2MVS capacity follows an ambitious multi-year roadmap (Janssens-Maenhout et al., 2020), addressing current limitations in observation availability for both insitu and satellite observations (Ciais et al., 2014), as well as indicating the need for significantly improving our modelling and data assimilation capabilities. The development of those components has been specifically targeted to enhance our capacity to separate anthropogenic CO_2 emissions from natural CO_2 variability. The CO2MVS, once operational, will be a key asset to quantify the effectiveness of policy-driven changes, supporting the European ambition of reaching Climate-neutrality by 2050, proposing a European Climate Law and a European Climate Pact (Delbeke and Vis, 2019).

Scientific studies of the carbon cycle tend to fall into two categories: "bottom-up" and "top-down".

In "bottom-up" emissions approaches, using process models and inventories, spatially heterogeneous information based on our knowledge of emission sources and their evolution over time can be combined. Bottom-up emission incorporate our knowledge of biological processes that drive the exchange of CO_2 between the atmosphere and the land and ocean. Inventory-based emissions tend to be more accurate for country-scale annual-mean estimates, especially for countries that have detailed procedures in place, but when these estimates are extrapolated to include much higher spatial and temporal resolution, uncertainties increase. Models based on our knowledge of biogeochemical processes, still have significant uncertainties, however improving those processes has not been a primary focus of the CHE project.

In "top-down" or "inverse" techniques, measurements of CO_2 abundance in space and time are used to infer the large-scale uptake and release of CO_2 at the surface. However, owing to the coarse spatial resolution adopted (coarser than 50 km), present-day inversion systems have clear difficulties in disentangling sources and sinks at local scales, and even bigger challenges in separating fossil fuel and other human-induced emissions from natural fluxes.

A synergetic solution is found through the combination of "top-down" and "bottom-up" approaches, as applied for instance in the framework of climate reanalysis (e.g., Hersbach et al., 2020) or biogeochemistry (Rayner et al., 2019). Further requirements are identified in the enhancement of resolution and transport accuracy (Agusti-Panareda et al., 2019) and by merging the available knowledge from emission inventories and process models with the increasing amount of observational data for the atmosphere and the Earth's surface. The Fossil Fuel Data Assimilation System (FFDAS; Asefi-Najafabady et al., 2014; Super et al., 2020a) and the Carbon Cycle Data Assimilation System (CCDAS; Rayner et al., 2005; Scholze et al., 2019) approaches represent significant efforts to bridge "top-down" and "bottom-up" approaches.

A mature and credible monitoring system for anthropogenic CO_2 emissions should be able to integrate all available information streams from Earth observations, inventories and activity data, and models of the atmosphere, land and ocean, which is a complex undertaking.

The CHE project started in October 2017, bringing together a consortium of 22 European partners and lasting for over 3 years. By the end of the CHE project, the global-scale developments have 1) demonstrated the high-resolution CO_2 modelling capability in global Nature-runs (Agusti-Panareda et al., 2021), 2) integrated updated global CO_2 sectoral emission datasets (Choulga et al., 2020), 3) constructed a new high-resolution (~10 km) input dataset for fossil CO_2 emissions since the 1960s (Jones et al., 2021), and 4) advanced the use of Ensemble-based uncertainty characterisation preparing the data assimilation step (McNorton et al., 2020). Sizeable advances at European scale include the realisation of high-resolution CO_2 emission inventories (Super et al., 2020b) that served also as exploratory studies of what can be achievable at global scale, where high quality inventories are made available. Similarly, the global modelling and data assimilation advances (Bousserez, 2019; Barré et al., 2020) had beneficial links and interactions, comparing the methodological work done over Europe and exploiting a wealth of dataset gathered within the VERIFY partner project (https://verify.lsce.ipsl.fr/).

CHE also supported some rapid response studies during the 2020 COVID-19 pandemic, estimating a 17% decrease in global daily CO_2 emissions during the initial outbreak phase (Le Quéré et al., 2020; Liu et al., 2020), which has stimulated advances in the use of human activity data for rapid and continuous assessment of CO_2 emissions (e.g., https://carbonmonitor.org). These results have been supported by EO-based estimations (Buchwitz et al., 2020; Chevallier et al., 2020; Weir et al., 2020; Zheng et al., 2020).

The CHE Horizon 2020 project ran from October 2017 to December 2020. As a Coordination and Support Action, CHE actively brought together European expertise to introduce a consolidated approach of building an operational anthropogenic CO_2 emission monitoring and verification support capacity. There were four main areas of work, covering:

1) Observations,
2) Emission inventories,
3) Modelling and
4) Inversion systems.

The three central questions that CHE addressed are:

- What does it take to have a combined "bottom-up" and "top-down" estimation system capable of distinguishing the anthropogenic part of the CO_2 budget from the natural fluxes?
- How can we make the first steps towards such a system that can use the high spatial and temporal resolution of satellite observations to monitor anthropogenic emissions at the required time scales?
- What does it take to transform a research system into a fully operational monitoring support capacity?

This paper summarises some of the key achievements towards the development of a CO2MVS prototype, as well as the definition of an implementation plan which includes requirements and priorities in consideration of the calendar described within the Paris Agreement and in the European Commission CO_2 Task Force reports (Ciais et al., 2016; Pinty et al., 2017; Pinty et al., 2019; the CO_2 blue, red, and green reports respectively, https://www.copernicus.eu/en/news/news/new-co2-green-report-2019-published). The CHE developments and findings have been transferred to a new project, which will develop a prototype Copernicus CO_2 Service (CoCO2 project, https://coco2-project.eu/) and will run from January 2021 to December 2023. This follow-on project has a particular focus on supporting the first Global Stocktake of the Paris Agreement to be held in 2023. It will have a particular focus on the implementation and readiness of both the monitoring prototype and the information product portfolio that can support an operational phase. This will be done in close coordination with the European Commission, nations that are party to the United Nations Framework Convention on Climate Change, and international stakeholders.

In the following sections a description of the methodology developed, and selected results, are presented to provide a synthesis of the key CHE achievements in this first phase of the CO2MVS development, which continues within the Copernicus CO_2 Prototype project and are embedded in the evolution of the Copernicus Atmosphere Monitoring and Climate Change Services (CAMS and C3S).

METHODOLOGY

In 2015, a first report from the European Commission CO_2 Task Force, Ciais et al. (2016), proposed a European support capacity for monitoring anthropogenic CO_2 emissions and concluded that a comprehensive observing system should be based on a combination of space-borne observations and ground-based monitoring networks.

Inverse transport modelling (Bergamaschi et al., 2018) still relies on the availability of *prior* fossil fuel CO_2 emission estimates and uncertainties, as well as prior biogenic fluxes and uncertainties, and provides *posterior* fossil fuel CO_2 emission estimates. However, inversions often do not integrate the full process knowledge and often neglect atmospheric transport uncertainties, which Schuh et al. (2019) have highlighted as a major source of bias in annual carbon budgets.

The global system used in CHE rely on the ECMWF Integrated Forecast System and the experience gained within the Copernicus Atmospheric Monitoring System Re-Analysis—CAMSRA (Inness et al., 2019). The capacity to assimilate a large amount of remote sensing data informative of atmospheric concentrations and optimally combined with atmospheric composition and transport modelling, is a clear advantage of the integrated approach developed in CHE, which extend this capability for generating a *posterior* fossil fuel CO_2 emission estimate, consistently integrating both Earth observations and process knowledge accounting for the uncertainties in each of the building blocks.

Building Blocks: Observations, Modelling, Assimilation, Uncertainty

The requirements for integrating Earth observation in an Earth System Model via data assimilation methodology, in the context of a CO_2 monitoring service, should account for the multiscale aspect of the problem (**Figure 1**). Multiscale in this context refers to both the spatial and temporal domains represented in a prototype system.

For the spatial domain a challenge of detection is inherently linked with the local nature of anthropogenic emissions as they emanate from stacks, cars, and buildings (point sources, <100 m scale). The resulting CO_2 in the atmosphere travels over hundreds of kilometres while interacting strongly with natural ecosystems (from 1 to 100 km), weather systems (from

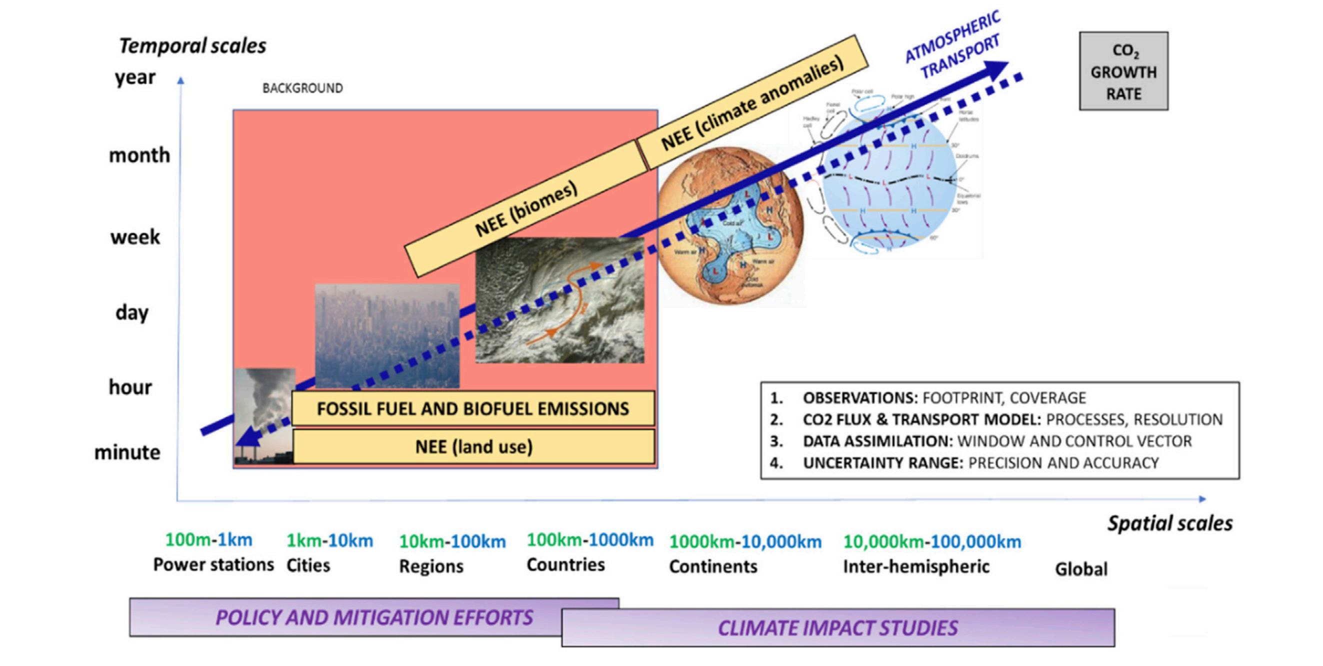

FIGURE 1 | Temporal and spatial scales of CO_2 monitoring from plumes to global CO_2 growth rate.

10 to 1,000 km) and eventually across the full hemisphere (>10,000 km) and the rest of the globe. Not one modelling system can capture all these scales, and strengths of global scale models thus need to be combined with other modelling approaches (e.g., Regional Models, Lagrangian, Gaussian plume, Large-eddy simulations).

In the temporal domain it is recognized that signals of anthropogenic emissions are stronger and easier to detect close to their source but get diluted at the typical boundary layer mixing time scale of 15–30 min (Broquet et al., 2018; Kuhlmann et al., 2019).

The key requirements within the CHE project stem from research done in the work packages dedicated to scientific advances and from connecting the specific requirements of the CHE Monitoring and Verification System prototype. These are detailed in the CHE deliverables Chevallier (2020, D5.2), Agusti-Panareda and Brunner (2020, D5.4), Peters and Krol (2020, D5.6), Scholze et al. (2020a, D.5.8), respectively, covering the Earth observations, the modelling components, the data assimilation methodology and the uncertainty characterisation.

The global monitoring system must allow us to separate the impact of anthropogenic emissions from the effect of the complex natural carbon cycle, while observation requirements may not yet be fulfilled (Ciais et al., 2014) for both the anthropogenic and biogenic components, since both emissions simultaneously affect atmospheric CO_2 concentrations.

Although observations from satellites, ground-based observation networks and aircraft provide CO_2 information at specific times and locations, alone they do not constitute a continental to global monitoring capacity across different time scales. Moreover, these observations mostly measure atmospheric CO_2 abundances at a given location, which is not directly informative of the underlying carbon emissions or uptake. Therefore, the use of atmospheric transport models or an Earth System modelling infrastructure is required to combine Earth observations (ground-based, aircraft and satellite) with detailed CO_2 emissions inventory data.

The impacts of the CHE project are all linked to its function as a bridge between the European Commission and its CO_2 Task Force, space agencies and related industries, the CO_2 science community, and the Copernicus Services. The capacity building aspects of CHE focused on strengthening the links between these sectors and using these to scope the required architecture of a future CO_2 emission monitoring system.

It is important to note that the CHE project's impact is not directly related to end users. The impact results from providing building blocks that will make possible future operational services, which will then serve several categories of end users. The future end-users can be found in the policy sector, the science community and the private sector, as outlined in the European Commission's CO_2 report. However, liaising with final end-users is also required in designing a system that can meet the needs by 2025 and 2030. The VERIFY project has already dedicated efforts towards end-user products and achieved two important syntheses for CO_2, and methane (CH_4) and nitrogen oxides (NO_x) (Petrescu et al., 2020a; Petrescu et al., 2020b; Petrescu et al., 2020). This work will continue in the CoCO2 project from 2021 on, with a handover of a new VERIFY synthesis in 2022, targeting 2021 emissions. Existing international efforts, such as the annual synthesis provided by the Global Carbon Project (e.g., Friedlingstein et al., 2020) provide extremely valuable science-consensus datasets complementary to the finalities of the CO2MVS that aims at monitoring applications.

Design Considerations on Scales, Species, Streams

The CHE prototype will encompass multiple scales, species and streams in order to support the global, regional and local information. The approaches consist of:

- 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 25 km to 100 m).
- 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.

CAPACITY BUILDING AND DEVELOPMENTS

Global Monitoring and Verification Support Capacity

The CHE prototype for the global MVS capacity aims at providing global integrated CO_2 emissions and concentrations at a resolution sufficiently high to enable the representation of large emissions and their evolution in the atmosphere. The availability of reliable CO_2 concentrations and their transport will provide lateral boundary conditions for regional-scale and local scale inversions. Moreover, the availability of ensemble-based CO_2 realisations (McNorton et al., 2020) will enable offline modelling and coupled assimilation efforts to refine emissions detection capabilities, adapted to the CO_2 long-lived atmospheric concentration (Bousserez, 2019). In parallel to the CO_2 developments, exploratory studies for the CH_4 (Barré et al., 2020) have shown the capability of the CAMS system for local emission detection.

The ECMWF Integrated Forecasting System (IFS) that supports the Copernicus Atmosphere Monitoring Service (CAMS GHG forecasts) is currently running globally at 9 km (high-resolution (HRES) configuration, a single realisation). The operational ensemble weather forecast suite runs at 18 km (ENS) initialised by an ensemble data assimilation (EDA) configuration, with 50 members (Buizza et al., 1999; Leutbecher et al., 2017).

The new High Performance Computing infrastructure will permit exploration of a combination of the ENS/EDA/HRES at around 9 km foreseen in 2023. Moreover, new initiatives supported by the European Destination Earth Initiative (https://ec.europa.eu/digital-single-market/en/destination-earth-destine) further explore the impact of horizontal and vertical resolution and of more sophisticated biogeochemistry, with the aim to attain a resolution of 4 km by 2025 and 1 km by 2030, thanks to advanced supercomputing infrastructure and software innovations aiming at building a digital twin of planet Earth (Wedi et al., 2020).

The global MVS will provide 1) a robust, reliable, timely system to support the Global Stocktake with monthly estimates of EO-driven CO_2 emissions and their uncertainties, and 2) a Regional MVS capacity (see below and **Table 1**), both well nested in a development plan that benefits from synergies with the other Copernicus services.

Hotspot Monitoring and Verification Support Capacity

Hotspot or point scale inversions will permit the monitoring of emissions at local scale, for those locations where observation availability enables the sampling of plumes. Point scale simulations will benefit from global and regional scales for the provision of boundary conditions and prior information. In return, the local scale knowledge can support the error characterisation for both the regional and global scale MVS, as they will need CO_2 emissions inventories as prior estimates. The question of model error characterisation was addressed using Large-Eddy-Simulations detailed in Klonecki and Prunet, (2020, CHE D2.8). The stochastic dynamics of the plume under turbulent conditions leads to spatio-temporal variability in concentrations of CO_2 emitted from point sources. This variability, which should be taken as a source of uncertainty for inversions based on episodic measurements from polar-orbiting satellites, was quantified at scales typical of CO_2 space-based measurements. Preliminary evaluation provided in Klonecki and Prunet, (2020, CHE D2.8) suggests significant turbulent-induced variability on XCO_2 at the scale of satellite measurements (of the order of 20%), with possible biases on flux retrieval if not properly taken into account. Work is foreseen to use Large-Eddy-Simulations for deriving a reliable model representation uncertainty for local scale transport of power plant plumes. Turbulent features not captured by the forward modelling used in the inversion/assimilation process can be parametrised using the Large-Eddy-Simulations dataset.

The study of well-known emission hotspots has demonstrated the synergy of satellite observations of CO_2 and NO_2 (Reuter et al., 2019) in the case of isolated sources. Assessing interannual variability of CO_2 emissions remains a challenge with the current satellite coverage (Buchwitz et al., 2020; Chevallier et al., 2020; Weir et al., 2020; Zheng et al., 2020). However, city-scale monitoring capability has great potential with the increased data quality and availability offered by the CO_2 satellite

TABLE 1 | Global and Regional Modelling Systems participating to the CO_2 prototype phase (from the H2020 CHE and CoCO2 projects).

Model	Institute/Consortium	Domain	Archived resolution			Meteorology Boundary Conditions
			horizontal	vertical	temporal	
IFS	ECMWF	Global	9 km	137 levels	hourly	N/A—boundary condition provider
TM5+OpenIFS	WU	Global	25 km	60 levels	hourly	ECMWF operational/reanalysis
TM5	WU/SRON	Global	3 x 2	60 levels	hourly	ECMWF operational/reanalysis
		Zoom	1 × 1	60 levels	hourly	
LMDZ	CEA	Global	3.75 × 1.90	39 layers	30 min	ECMWF operational/reanalysis
GEOS-Chem	University of Edinburgh	Global	2.0 × 2.5	47 levels	hourly	GEOS-FP/MERRA-2
		Zoom	0.25 × 0.3125			
CCFFDAS	Lund University, iLab	Global	0.1 × 0.1	—	weekly	ECMWF operational/reanalysis
		Local	2 km	—	hourly	ECMWF/WRF
CHIMERE	CEA	Regional	1–2 km	29 layers	hourly	ECMWF operational/reanalysis
COSMO-GHG	EMPA	Europe	5 km	60 levels	hourly	ECMWF operational/reanalysis
		Regional	1 km	60 levels	hourly	
LOTOS-EUROS	TNO	Europe	5 km	20 levels	hourly	ECMWF operational/reanalysis
		Regional	1 km	20 levels	hourly	COSMO or WRF
ICON-ART	DWD/MPI-M/KIT-IMK	Europe	6.5 km	60 levels	hourly	global ICON and ECMWF
		Regional	2.5 km	65 levels	30 min	regional ICON and ECMWF
MICRO-HH	WU	Local	1—100 m	—	—	global or regional model

mission (Meijer et al., 2020) as demonstrated for the city of Berlin by Kuhlmann et al. (2019, 2020). While the CO_2 monitoring capacity brought by CO_2 Monitoring mission will be a key asset of the future CO2MVS (e.g., greater accuracy of detection, larger swath, higher spatial resolution and constellation of satellites), presence of clouds and large amounts of aerosol-load still pose challenges to the observational coverage in some areas. These caveats, related to observability, will result in higher uncertainties. Expanding ground-based observing networks should therefore be among the actionable responses, in agreement with recommendations by Chevallier et al. (2020). There are however also caveats in representation of processes that need sufficient resolution and precision (Agusti-Panareda et al., 2019) to be more directly comparable to the CO_2 Monitoring mission observations.

A data assimilation system that would just target one of the scales involved in natural and anthropogenic CO_2 variability would not capture the integrated emissions over larger areas. It would thus require continuous observations almost everywhere, which is not feasible even with new (satellite) instruments and techniques. The integral of CO_2 emissions and uptake is moreover a very useful constraint to quantify changes in biospheric uptake and release over ecosystem/country scales, needed to understand the annual carbon balance. A system that can combine scales from minutes up to weeks/months would thus represent the best of both worlds. Hereafter the key advances in each of the building blocks are discussed.

Earth Observations Developments

CO_2 observations of fluxes and concentrations with other types of Earth observation data such as radiocarbon, NO_2, oxygen, solar-induced fluorescence and carbonyl sulphide are reviewed in Chevallier (2020, CHE D5.2). These are clustered in satellite CO_2 and non-CO_2, ground-based remote sensing, *in situ* and flask-sampling observations. The relevant information from the Copernicus CO_2 Monitoring Mission Requirements Document and from the three reports of the Copernicus Expert group and of the CO_2 Task Force is included. Research needs for the identification of the role of each relevant Earth observation type in the Copernicus CO_2 support capacity system are identified, for data streams currently available. The synthetic satellite data instead aim at supporting studies for CO_2 Monitoring mission satellite constellation and are detailed in Strandgren, (2020, CHE D2.5). From experience gained within CHE and CAMS, the NO_2 and Solar Induced Fluorescence (SIF) satellite-based data are identified as global-coverage Earth observation information with currently more direct usability for data assimilation purposes. *In situ* observing capability is paramount to Evaluation and Quality Control of the CO2MVS. Sizeable advances in the Earth observations capability covering both satellite-based remote sensing (e.g., Copernicus Sentinel-5P, NASA OCO-3) and the ground-based network (e.g., the TCCON—Total Carbon Column Observing Network, the FLUXNET micrometeorological sites and the ICOS—Integrated Carbon Observation System sites) are documented in (Ciais et al., 2014).

Modelling Developments

The modelling and prior components, subdivided in atmospheric transport from both resolved transport (advection schemes) and unresolved sub-grid processes (convection and turbulence), biogenic fluxes and anthropogenic emissions, are reviewed inAgusti-Panareda and Brunner (2020, CHE D5.4). The high-resolution regional nature runs, nested in the European runs (described in Haussaire et al. (2020), CHE D2.4), are themselves nested in the global Tier-1 runs performed with the ECMWF/CHE-CAMS system (described in Agusti-Panareda (2019), CHE D2.2). These simulations are produced using two separate models, COSMO-GHG and LOTOS-EUROS. COSMO-GHG is used for both the meteorology and tagged tracers of multiple anthropogenic and biogenic sources. The meteorological outputs

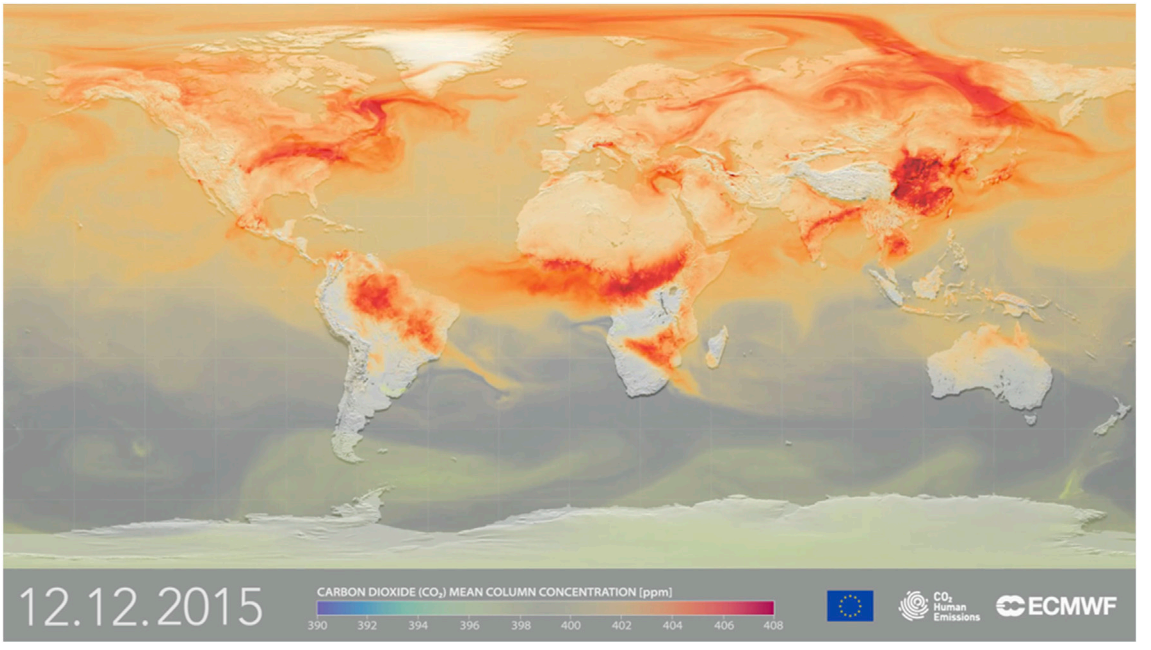

FIGURE 2 | Examples of the CHE Nature Run Tier-2 CO_2 concentrations valid for the December 12, 2015 obtained by global simulations with the ECMWF-IFS. Video for the whole 2015 available at https://www.che-project.eu/news/year-atmospheric-co2-variability-time-paris-agreement.

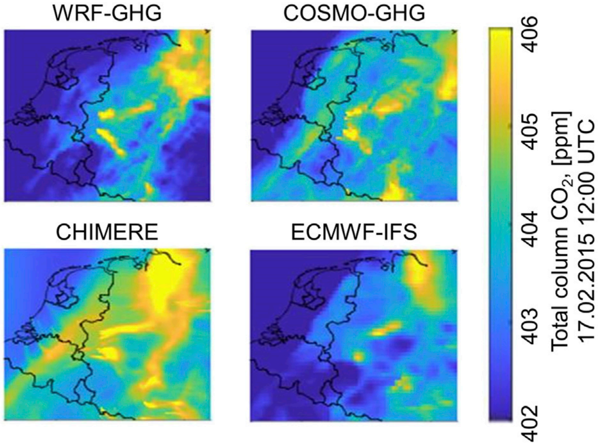

FIGURE 3 | Examples of CHE European regional CO_2 mole fractions valid for the February 17, 2015, centred over Berlin (Germany) with a focus on stacks from industry and power plants obtained by simulation with WRF-GHG, COSMO-GHG and CHIMERE (see **Table 1**), and comparison with the ECMWF-IFS.

drive the offline model LOTOS-EUROS, which computes reactive trace gases and aerosols on top of the tagged tracers. A comparison of the different transport models and prior datasets is included in Agusti-Panareda and Brunner (2020, CHE D5.4) to assess the different capabilities of the models and priors used to perform the CHE library of simulations. The Tier-2 global nature runs (Agusti-Panareda et al., 2021), see **Figure 2**, constitute a step improvement with respect to the Tier-1 runs, in both atmospheric transport and surface emissions, and demonstrate the incremental improvement cycle that will support the CO2MVS capacity. The lessons learnt on the key CO_2 modelling aspects span from the importance of high spatial resolution and accurate atmospheric transport (Agusti-Panareda et al., 2019) to the importance of specifying a vertical profile for emission sources not released at the surface level (Brunner et al., 2019), as in the case for industries stacks. An example of the European regional simulation is provided in **Figure 3** to illustrate the differences across systems, that reflect difference in spatial resolution, handling of processes, and choice of CO_2 inventory dataset.

Data Assimilation Developments

The data assimilation methodologies for CO_2 distinguish in online 4D-Var, offline 4D-Var, online EnKF, offline EnKF, offline analytical and hybrid ensemble Var varieties, which are reviewed in Peters and Krol (2020, CHE D5.6). The differences between direct flux estimation (transport inversion) and the inclusion of models for fossil fuel emissions (FFDAS) and biospheric fluxes (CCDAS) are discussed with their implications on the control vector configuration, and the error covariances statistics, along with examples of existing inversion systems. A configuration for global and regional inversions is presented. This includes a multi-scale and multi-species data assimilation system that targets anthropogenic CO_2 emissions and is capable of ingesting multiple streams of observations, including satellite observations.

A hybrid 4D-Var ensemble approach (Bousserez, 2019) implemented in an online transport model, and operated within the Numerical Weather Prediction environment (Bonavita et al., 2016), was identified as a fundamental

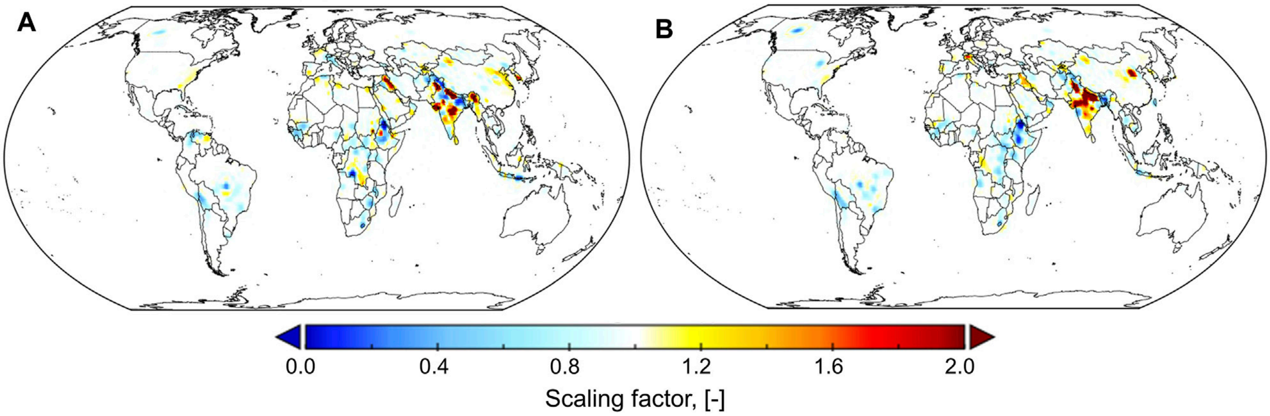

FIGURE 4 | (A) Daily unitless scaling factors for CO emission on 29-05-2019 based on augmented state 4D-Var assimilation of MOPITT and IASI CO observations; **(B)** same as a) but on 30-05-2019.

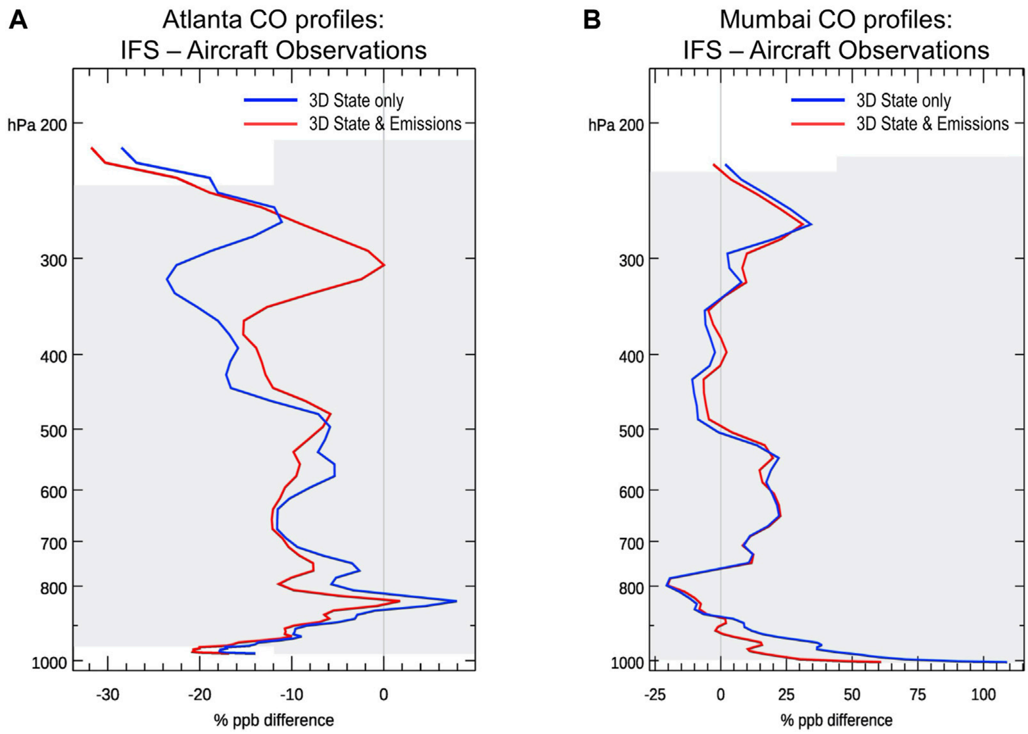

FIGURE 5 | Relative difference (model-observation) in CO concentration between IFS analysis and aircraft measurements over Atlanta **(A)** and Mumbai **(B)** for a reference state-only (blue) and a joint atmosphere/surface-emission analysed state (red).

building block towards extending the Data Assimilation system capability to using constraints from multiple tracers and long 4D-Var windows for joint atmospheric state and surface fluxes optimisation. This methodology accommodates operational constraints (e.g., computational efficiency, seamless integration into current Data Assimilation system) by combining existing ECMWF products, such as the adjoint-based 4D-Var algorithm (Courtier et al., 1994) and ensemble simulations (Buizza et al., 1999; Leutbecher et al., 2017).

Additionally, a novel approach to integrate multi-scale and multi-model posterior emission products (i.e., regional, local inversions) into the global IFS prototype has been proposed that consists of directly assimilating those external outputs as observations. Such integration effort would help improve the flow of information across different CO_2 inversion products and equally applied to CO and CH_4. This will facilitate interpretation of the data assimilation results and enhance usefulness for users and stakeholders by providing a unified framework for Carbon

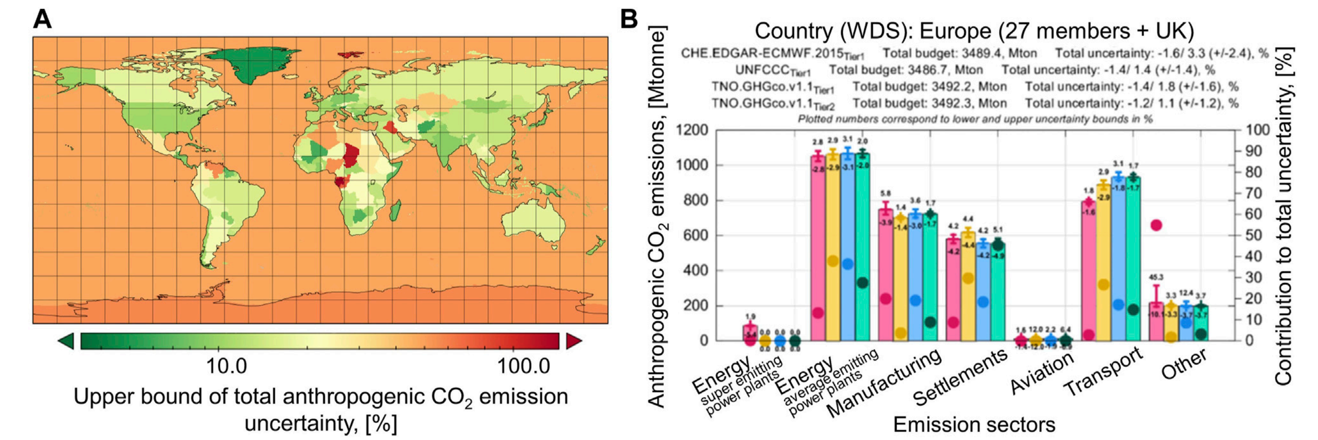

FIGURE 6 | Upper bound of global annual anthropogenic CO_2 emission uncertainty, in % (logarithmic scale) **(A)**, and illustration of European sectoral emissions with uncertainties bounds (b) from Choulga et al. (2020). In the example of sectoral emissions Europe 27 + United Kingdom is shown **(B)**, with Energy production subdivided in super-emitters S and average emitters A, and four main emission sectors are represented for Manufacturing, Settlement, Aviation and Transport, with all remaining emission sources clustered in "Other".

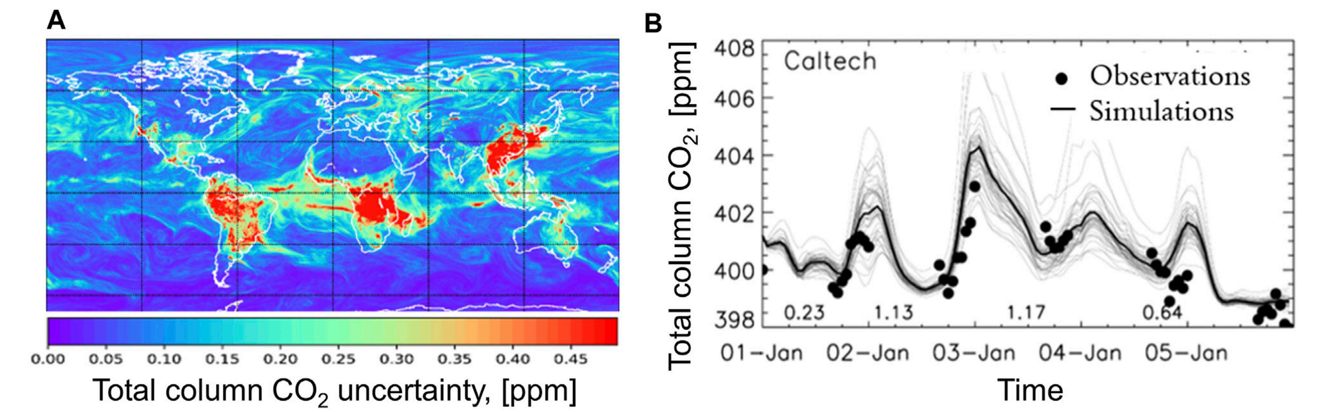

FIGURE 7 | Total column CO_2 global model error from a 50-member IFS ensemble **(A)** accounting for uncertainties in meteorological initial conditions, model physics, anthropogenic emissions and the biogenic feedback after a 10-days simulation in January 2015, and **(B)** illustration of the CO_2 ensemble spread at Caltech, United States compared with Total Carbon Column Observing Network (TCCON) observations with grey thin lines represents each of the single ensemble member simulations, from McNorton et al. (2020).

inversions. A preliminary short-window 4D-Var prototype has been developed within the CHE project, building on previous CO_2 data assimilation implementation in the IFS (Engelen et al., 2009; Massart et al., 2016; Massart et al., 2020) and aided by recent infrastructure for an augmented control variable. **Figure 4** shows the geographical distribution from a CO emission inversion using the new prototype. The CO emission scaling factors show sizable corrections over Asia, Africa, and South America, while smaller localised corrections can be seen over Europe, reflecting the better knowledge in the prior emission inventories over those developed countries. Looking at vertical profiles of CO concentration in **Figure 5** significant improvements are obtained by the 12-h analysis compared to the modelled CO concentrations prior, evaluated with independent aircraft profile observations, both in the lower and upper troposphere.

Uncertainty Characterisation Developments

The components in the sub-sections above are all characterised by uncertainties in space and time that need to be realistically represented and that are detailed in Scholze et al. (2020b, CHE D5.8). The posterior uncertainty is evaluated in Observing System Simulated Experiments and in the Quantitative Network Design studies, within the CHIMERE and CCFFDAS systems, respectively. The CCFFDAS allowed to assess several design aspects of the upcoming MVS capacity as part of the Copernicus CO_2 Monitoring mission.

The assessment was based on the Quantitative Network Design technique (Kaminski and Rayner, 2017) and quantified the mission's performance in terms of the posterior uncertainty in

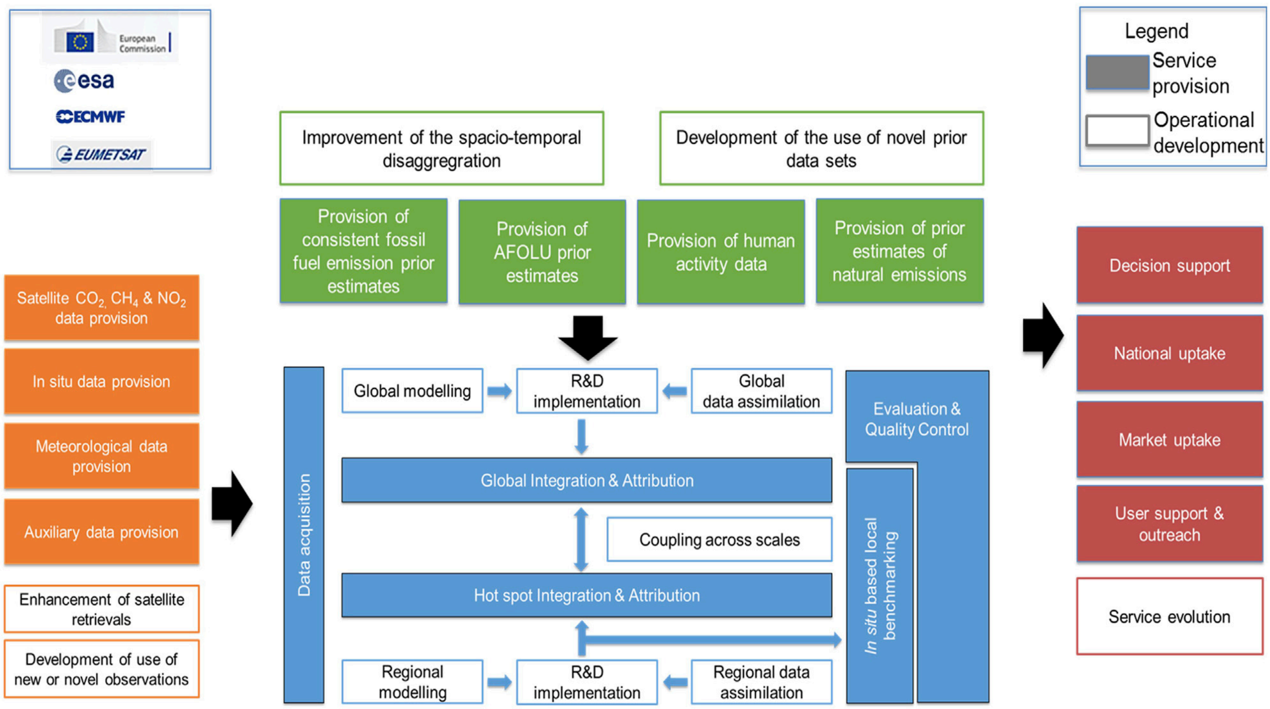

FIGURE 8 | Schematic of the anthropogenic CO2 emissions Monitoring and Verification Support capacity (CO2MVS) as developed in the CHE project and adopted by the CO2 Monitoring Task Force. The foreseen service provision elements are depicted by the coloured boxes, while the required continuous development of the operational services is depicted by the white boxes.

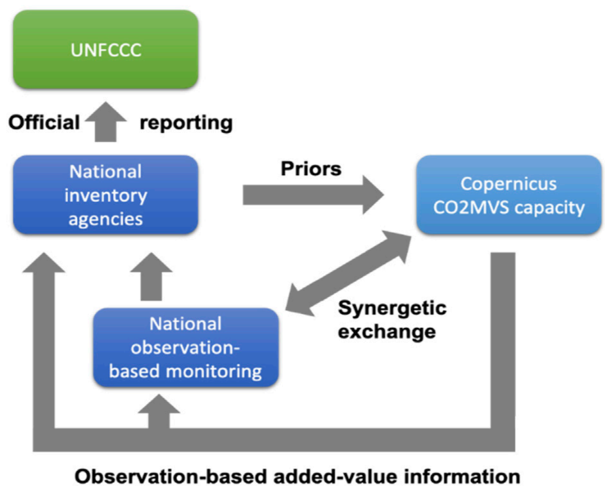

FIGURE 9 | High-level schematic of the envisaged interaction between the Copernicus CO2MVS capacity and countries as part of the UNFCCC reporting process.

the total CO_2 emissions classified into two sectors, one for electricity generation and the other for all other emissions denoted as the "other" sector. Analysis of two different observing networks, ground based *in situ* observations and satellite based total column observations, in a range of configurations is detailed in Scholze et al. (2020a, CHE D3.6).

We also have numerically assessed how anthropogenic CO_2 emissions are depending on country of origin based on IPCC 2006 Guidelines and its Refinement of 2019 (Choulga et al., 2020), see **Figure 6**. These uncertainties gridded globally at 36 and 9 km resolutions, provided prior uncertainty information for CO_2 ensemble runs (McNorton et al., 2020), see **Figure 7**, and

TABLE 2 | Proposed CHE prototype configurations for global, regional and local domains.

Operational System	Domain	Stream	Recommendations
IFS/Global Models	Global	NRT (Near Real Time, as in the Forecast mode) + BRT (Behind Real Time, as in Reanalysis mode)	Resolution + Accuracy + Timeliness to provide Satellite Monitoring Capabilities relevant for CO_2 Monitoring mission and Modelling Boundary Conditions for the Regional/Local efforts. Inclusion of activity data and process knowledge
Land-Atmosphere Model (LAM) type	Regional	BRT	Linkage to global enabling European high-quality inventories and *in situ* coverage for Evaluation and Quality Control efforts, see **Table 1**
Large-Eddy-Simulations (LES) types	Local	BRT	Linked to regional/global for identified hotspots and to characterise model uncertainty and improve transport modelling

Tier-2 nature runs (Agusti-Panareda et al., 2021), see **Figure 2**, respectively.

The atmospheric uncertainty in CO_2, shown in **Figure 7**, is the combined effect of anthropogenic emission uncertainties (largest over emission hotspots in eastern China, and smaller signals over North America, Europe and the Middle East), as well as biogenic emission uncertainties in areas with high net ecosystem exchange, such as the Amazon and Southern Africa.

While a full representation of biogenic related uncertainties (e.g., structural vegetation properties, land-use-change) is not yet developed, this study has highlighted the importance of accounting for flow dependent errors and the interplay of biogenic and anthropogenic CO_2 emissions.

Also, as part of the CHE project, Jones et al. (2021) have produced a gridded global dataset of CO_2 emissions and their uncertainty at 0.1-degree resolution to be used as a prior for multi-decadal runs of "top-down" models (e.g., Friedlingstein et al., 2020), where uncertainties respect the country and sector of origin, relevant for the target of consistent climate reanalysis (Dee et al., 2014).

IMPLEMENTATION PRIORITIES

Among the CHE significant achievements there are the preparation steps needed for the first global stocktake of the Paris Agreement, which have been documented with identified priorities along with the prototype system design as briefly detailed in the two following sub-sections.

Support the 2021 Global Stocktake in 2023

This set of recommendations focuses on the follow-on work to CHE, that will be taken up in the CoCO2 project:

- A "step-wise" approach to the MVS prototype will be followed according to the priorities defined in Chevallier (2020, CHE D5.2), Agusti-Panareda and Brunner (2020, CHE D5.4), Peters and Krol (2020, CHE D5.6), Scholze et al. (2020b, CHE D5.8) to achieve a prototype by 2023.
- Three scales: global, regional, and hotspots will have different setups and observation/modelling possibilities. The global scale system will serve the regional/local scale by providing boundary conditions. Regional/local systems will serve as important benchmarks for the global CHE prototype.
- The modelling resolutions of the first CHE prototype will focus on the highest resolution of 9 km globally with support from an ensemble system to characterise uncertainties. An exploratory 4 km system will be tested.
- An Near Real Time/early-warning system (for satellite monitoring, and attribution studies) with all available Near Real Time observations (L2 and/or radiances) supported by a multi-scale data assimilation approach will aim at ensuring consistency across scales.
- A delay-mode reanalysis (with focus on the Global Stocktake) with best quality observations ancillary/ inventories will be developed by 2023 and applied to 2021.
- CO2MVS demonstrations and case studies will benefit from application to CO_2, CO, and CH_4.
- The Benchmarking with observations that are not used in the assimilation steps will be essential for Evaluation and Quality Control.
- Cross-comparison between systems will provide a way forward to gain further insights on the prototype.

Proposed Prototype Configurations

The proposed configurations to cover the domain and stream are reported in **Table 2**. The CO2MVS service structure, outline in **Figure 8**, will operate in interaction with the relevant agencies, as outlined in **Figure 9**. More details are provided in the **Supplementary Material**.

CONCLUSION

This paper summarises and discusses the CHE project advances, linking CO_2 service elements with the scientific work and outlining the preoperational setup that will be further developed in the CoCO2 project 2021–2023.

CHE has advanced on the development of a European CO_2 monitoring and verification support capacity for anthropogenic CO_2 emissions: enhancing the global, regional and local CO_2 simulation capabilities, with focus on anthropogenic source representation, moving towards a global CO_2 inversion capability at high resolution to connect atmospheric concentrations to surface emissions, and demonstrating the use of Earth observations (satellite and ground), as well as proxy human activity data, to constrain uncertainties and to enhance the CO_2 monitoring timeliness, and to continuously evaluate its quality.

The timeliness of the monitoring suite will especially depend on the availability of the input satellite data (e.g., current commitment from ESA and EUMETSAT for the CO_2 Monitoring mission is 24 h after sensing), but also on more detailed user requirements. The exact schedule for a reanalysis inclusive of the CO_2 discussed here, will also have to be defined and tested based on user requirements and reprocessing capabilities by EUMETSAT. Furthermore, all service provision activities at ECMWF will have to be linked to and coordinated with the contracted service provision activities as well as with other relevant activities within CAMS (e.g., NO_2). All these aspects are a critical element of the ramp-up phase and will require significant time and resources. ECMWF has gained expertise with the implementation and operation of the current C3S and CAMS services, which will benefit the introduction of the CO2MVS in an operational environment. A track record of successfully converting science into operational services is key to engage European expertise implementing a CO_2 Copernicus service element.

The CoCO2 project will continue and expand the CHE developments with particular focus on supporting the first Global Stocktake of the Paris Agreement and advancing the implementation and readiness of both the monitoring prototype and the information products portfolio that can support an operational phase, in close coordination with the European Commission, the United Nations, and National and International stakeholders.

TEAM LIST

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DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/**Supplementary Material**, further inquiries can be directed to the corresponding author.

AUTHOR CONTRIBUTIONS

GB prepared the manuscript with contributions from all co-authors. The CHE team is acknowledged for the comments to the draft manuscript and for the development contributions.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/frsen.2021.707247/full#supplementary-material

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Conflict of Interest: PP was employed by SPASCIA

The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.