Progress report on service elements for CO_2 emission and transport models integration

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et al.

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D5.3 Progress report on service elements for CO2 Emission and Transport Models Integration

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1 Executive Summary

The CHE prototype is designed to estimate CO_2 emissions using a modelling framework to link all the CO_2 relevant observations with prior knowledge of the anthropogenic emissions and other natural fluxes that affect the observed atmospheric CO_2 signal. The modelling aspects include atmospheric transport, atmospheric chemistry and land surface and ocean biogeochemical and transport processes, as well as statistical models of anthropogenic emissions of CO_2 and co-emitted species based on human activity data. A multi-scale, multi-species and multi-stream approach is required to target the various types of CO_2 emissions and natural fluxes, and their wide range of scales from point sources to cities, regions/ecosystems and countries. Different transport schemes suited for the different applications from local to global scales are listed and their challenges are described. The various approaches to estimate biogenic fluxes and anthropogenic emissions that serve as prior information are reviewed with their strengths and weaknesses. A comparison of the different transport models and prior datasets is proposed to assess the different capabilities of the models and priors used to perform the CHE library of simulations.

2 Introduction

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 CH_4 between the Earth surface and the atmosphere with the use of observations (mostly in the atmosphere), models and prior information, as well as their uncertainties to leverage the different sources of information. The system is designed to support the Paris Agreement and follows the directive of the European Commission CO_2 Task Force (Pinty et al., 2017). The general strategy and rationale for the CHE prototype is provided in CHE 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 emission from point sources (power stations or industrial facilities), cities and countries using different model domains from global to regional and to local 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 (NRT) 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.

This report focuses on the modelling and prior components of the prototype. It complements the reports on Earth observations (CHE D5.1), data assimilation methodology (CHE D5.5) and uncertainty representation (CHE D5.7). Modelling and prior information encapsulate our current knowledge and understanding of physical (e.g. atmospheric transport), biological (e.g. photosynthesis and ecosystem respiration) and chemical processes (affecting co-emitted reactive species like NO_x, CO and CH_4), as well as human activity (e.g. fossil fuel energy production) that control the CO_2 exchange between the earth surface and the atmosphere.

This knowledge and information are crucial to fill the gaps in the observing system and connect observations with the CO_2 emissions and natural fluxes that need to be monitored.

The different model components and prior information of the emissions are shown in Figures 1 and 2. Some model components will play a role of observation operators (linking observations to CO_2 fluxes) and others will provide prior flux information in the data assimilation process described in CHE D5.5. The individual components can be either coupled or integrated together in the forward model configuration which propagates the information from the surface fluxes to the atmospheric CO_2 concentrations forward in time. In an offline system (Figure 1), the components are connected through input/output streams. The components are designed to be run separately without allowing for feedbacks. In online models (Figure 2) the components are fully integrated, ultimately becoming an Earth System Model. They share the mapping and input data, ensuring consistency between components and they can interact with each other, allowing for the representation of complex feedbacks. The degree of coupling or integration can vary between different models and configurations. Offline models are faster and not as costly to run as ESMs. Whereas online models based on prognostic equations can be used to predict the atmospheric CO_2 state forward in time from days (e.g. Agusti-Panareda et al., 2014) to decades (e.g. Friedlingstein et al., 2006).

Section 3 provides a detailed description of the essential components in the model and prior information for the prototype. The strategy for their implementation in the protype is outlined in section 3.1. The model components are grouped into atmospheric transport which affects all the atmospheric tracers (section 3.2) and prior fluxes and other processes (e.g. chemistry) which vary depending on the species (section 3.3). Model development is essential to ensure a more accurate interpretation of observations and a more accurate representation of prior information. For example, the hourly to daily variation of the CO_2 signal from biogenic fluxes and anthropogenic emissions is often correlated with the signal from atmospheric transport. These processes need to be understood and represented in the model to be able to interpret the high temporal and spatial variability in the observed CO_2. In this report, the different challenges are addressed by going through the different components in the model, listing their options for implementation in the prototype and the approaches to evaluate their accuracy. Sections 4 and 5 list the immediate requirements for the implementation of the prototype by 2023 and the research needs for the next 5 to 10 years. Section 6 concludes with a list of the work planned for the final report due in September 2020.

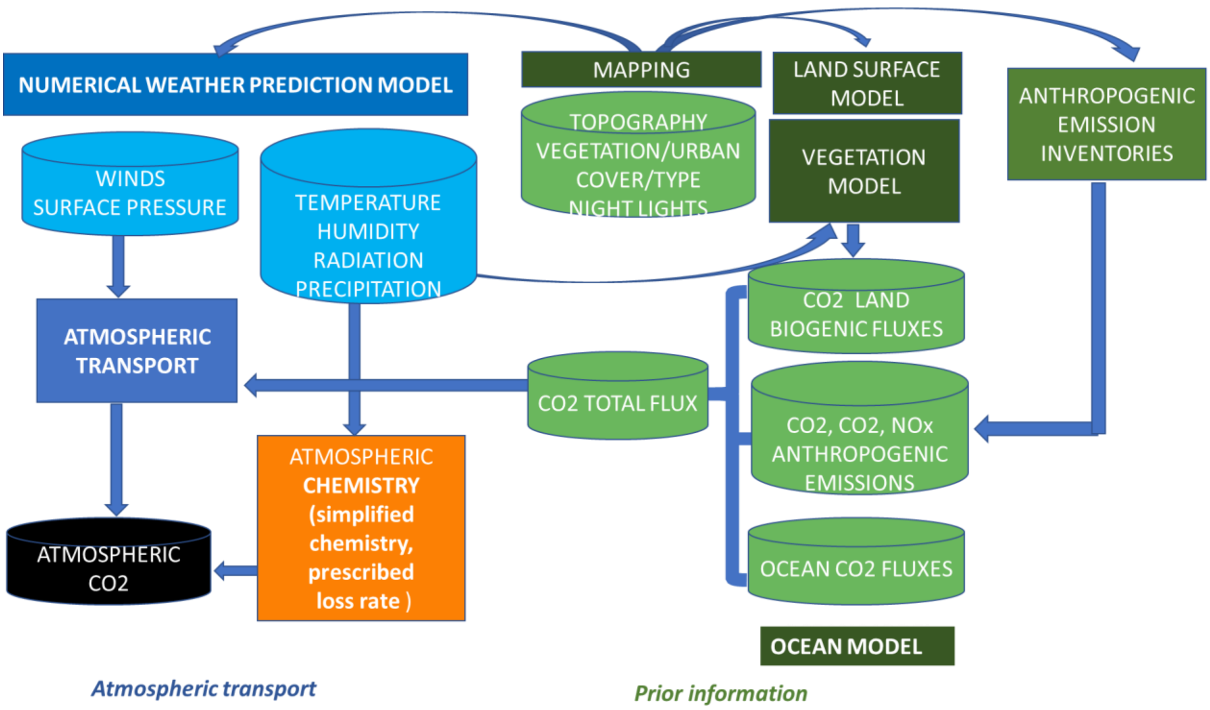

Figure 1 Offline approach to modelling and prior information provision with different components originating from independent models or products.

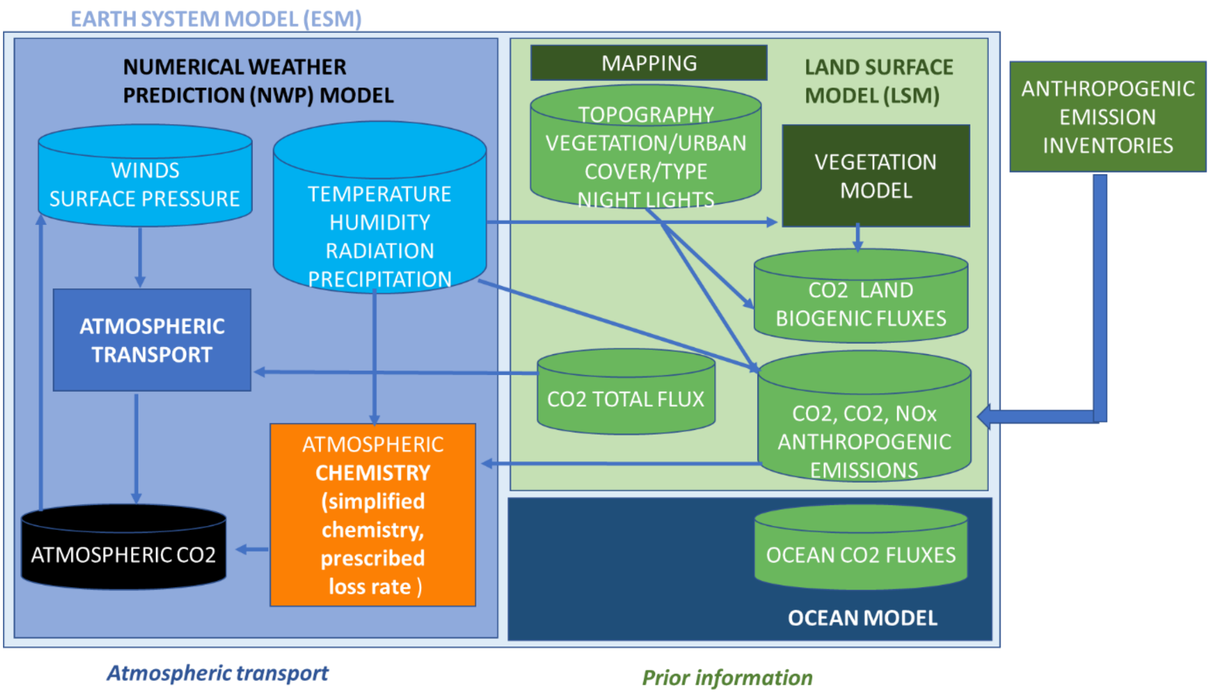

Figure 2 Online approach to modelling and prior information provision with different components integrated in Earth System Model.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverables

In this report we will describe the strategy to represent the modelling and prior information aspects in the monitoring system. The different options for the modelling of transport and prior products for operational use and for research and development purposes are described. Finally, priorities for implementation by 2023 and for longer term research needs will be outlined, together with future plans for the final report, including the evaluation of the transport models and prior CO_2 fluxes used in the CHE nature runs.

2.2.2 Work performed in this deliverable

Synthesis of modelling aspects in CHE, CAMS, VERIFY and other ESA-funded projects as well as literature on carbon cycle and transport models.

2.2.3 Deviations and counter measures

Not applicable.

3 Modelling and prior components of the CHE prototype

3.1 Implementation strategy

The design of the CHE prototype requires the assessment of the different options for each component which depends on an implementation strategy. The implementation strategy for modelling and provision of prior information is based on three approaches:

- **HIGH RESOLUTION AND MULTI-SCALE CAPABILITY**

Given the wide range of scales of CO_2 signal (from point sources to hemispheric gradients), it is crucial to approach the problem with a high resolution and multi-scale monitoring capability (see D5.9). For prior anthropogenic emissions, point sources merit to be treated separately (e.g. power stations). Their total annual budget is usually well known and thus, it is distributed to the point source first, before applying a temporal scaling to modulate its variability on sub-annual timescales. The plumes from point sources will also require dedicated plume models, as global and regional models cannot resolve such small scales.

EXAMPLES: From global Numerical Weather Prediction (NWP) models to plume dispersion models focusing on hotspots

- **ONLINE AND COUPLED MODELLING CAPABILITY**

The observed atmospheric signal is a result of the interaction between the signal of the flux and the atmospheric transport. Because both fluxes and transport have a high spatial and temporal variability, they often co-vary. Thus, it is crucial to represent this co-variability in space and time (e.g. rectifier effect). Biospheric fluxes depend on meteorological conditions, but also anthropogenic emissions are influenced by meteorology (e.g. heating demand, traffic). Thus, modelling the fluxes, meteorology and atmospheric transport online in a coupled mode is desirable because it allows an optimal consistency between components and it also has the potential to transfer information from one component to another (e.g. atmospheric concentration to winds). For small-scale plumes, coupled data assimilation will be required to modify winds according to the observed plume. Otherwise, the MVS will be limited to plume imaging and mass-balance methods.

EXAMPLES: Coupled NWP models, Earth System Models (ESM)

- **OFFLINE MODELLING CAPABILITY**

As the focus is on trends on decadal scales, it is crucial to be able to run long simulations. The interactions between the different components can also create difficulties in the attribution and calibration of parameters. Therefore, it is also crucial to develop an offline modelling capability as a research tool and to have the potential of running long re-analysis simulations at lower cost. Offline transport models also offer the possibility to use long DA windows as atmospheric CO_2 and fluxes preserve the linearity assumption used in most DA methodologies. Offline models could also be used to perform controlled experiments for developing specific processes, e.g. calibration of model parameters.

<u>EXAMPLES</u>: Chemical Transport Models (CTMs), emission inventories, data-fusion products, offline land surface models, plume dispersion models

Evaluation of the different modelling and prior components is required to estimate their uncertainty for data assimilation purposes (see CHE D5.5, CHE D5.7), but also to assess priorities in the implementation of new model developments and new improved priors:

1. Sensitivity experiments to assess impact of priors, their temporal and spatial distribution and their interannual variability or model changes on the atmospheric signal
2. Model/product inter-comparison to benchmark new developments/priors
3. Evaluation with indirect observations (e.g. atmospheric observations)
4. Evaluation with direct observations (e.g. FLUXNET data)

3.2 Atmospheric transport

Atmospheric transport models act as operators that link the atmospheric CO_2 observations to the surface fluxes. Modelling atmospheric transport of CO_2 is not trivial. The high heterogeneity in the surface fluxes lead to complex horizontal and vertical gradients in the atmosphere. As CO_2 is a passive tracer, any small errors coming from meteorological input, numerical representation of transport processes or temporal spatial resolution can accumulate and become as large as the signal (e.g. atmospheric growth rate of around 2ppm). Many efforts have been devoted to transport inter-comparison studies (e.g. TransCom experiments by Rayner and Law, 1995; Law et al., 1996; Gurney et al., 2003; Patra et al., 2008, Law et al., 2008, Stephens et al., 2007; Karion et al. 2019). Despite the recent decrease in the spread between the transport models (Gaubert et al, 2019), transport still remains a major source of uncertainty in atmospheric CO_2 inversions (Basu et al., 2018).

There are two main approaches in the representation of transport from large-scale to local plumes:

- Offline transport (Chemical Transport Models): More flexibility in terms of options, but requires pre-processing of winds, in particular vertical wind is diagnosed through bottom-up mass balance. Yu et al. (2018) presents some of the limitations for the offline transport models.
- Online transport (Numerical Weather Prediction models extended with a module allowing flexible definition of (passive) tracers): Emphasis on consistency and high-resolution capability, instantaneous (time step) coupling, direct computation of winds

and parameterization of unresolved convective and turbulent mixing, as well as potential access to other ESM components such as land and ocean. Online models can consider feedbacks between components and offer the possibility of joint atmospheric composition - meteorology data assimilation (e.g. assimilation of CO_2 plume observations affecting simulated winds).

3.2.1 Eulerian transport models

Advection schemes

The horizontal and vertical transport that is resolved by Eulerian models is performed by advection schemes using wind information from an NWP model or NWP analysis. There are two main approaches:

- **Eulerian advection schemes** are commonly used by offline chemical transport models (e.g. CHIMERE, Gavete et al. 2012) They are also common in mesoscale NWP models such as WRF (Wang, 2009) or COSMO (Schneider and Bott, 2014) and global NWP models (e.g. nonhydrostatic finite-volume dynamical core IFS, Kühnline et al., 2019).The timesteps are restricted by maximum Courant–Friedrichs–Lewy (CFL) number criterion, implying short timesteps. They can be designed to conserve mass locally.
- **Semi-Lagrangian (SL) advection schemes** are commonly used in global NWP models and online tracer transport models e.g. IFS (Diamantakis, 2014), COSMO-GHG (Liu et al. 2017). They are very efficient for multi-species transport, with unconditional stability permitting long timesteps. However, they do not necessarily conserve mass locally, although solutions exist (Zerroukat, 2010). New versions of the scheme are being tested that are almost mass conservative (e.g. SL continuous mapping about the departure point in the IFS, see Malardel and Ricard, 2015).

Benchmarking:

Test for positive definiteness, shape preservation (preserving monotonicity and/or convexity), amplitude preservation (low degree of numerical diffusivity), mass conservation.

Unresolved transport: convection and turbulent mixing parameterisations

Small-scale transport associated with convective and turbulent mixing processes cannot be resolved by global and regional models running at horizontal resolutions of 10 to 1km and therefore requires a parameterization scheme:

- Convective transport is based on NWP parameterizations designed to transport water tracers, heat and momentum with a mass flux formulation. Transport models can compute the convective transport by calling the NWP convection schemes or by using the mass fluxes archived by NWP models (e.g. Feng et al. 2011). The role of the convection scheme depends on the model resolution.
- Shallow and deep convection are very efficient processes for the ventilation of tracer from the Planetary Boundary Layer (PBL) to the free troposphere (e.g. Yu et al.,

2018, Belikov et al., 2013). Transient convection and PBL ventilation can be sensitive to temporal resolution of the model (Yu et al., 2018).

- Turbulent mixing distributes the anthropogenic emissions and natural fluxes from the surface throughout the PBL. Under stable conditions with low wind speeds, tracers remain trapped close to the surface. Modelling turbulent mixing under such conditions is very challenging (Sandu et al., 2013). Parameterizations of turbulent mixing can have a large impact on the wind speeds (Sandu et al. 2013), CO_2 concentrations (McGrath-Spangler et al., 2015) and plume dispersion from emission hotspots as shown by Large Eddy Simulations (LES, e.g. Gaudet et al., 2017). It is therefore crucial to improve the vertical profiles of winds and turbulence within the PBL to be able to model the plumes from hotspots (Karion et al. 2019).
- The coupling of shallow convection and turbulent mixing is an important aspect of NWP (water and energy cycles) and tracer transport (affecting long-range transport of tracers, including CO_2). ECMWF is addressing this coupling with the development of a more integrated physical parameterisation approach in the IFS which will be tested with CO_2 and other tracers.

Benchmarking: Use radon to assess convection and PBL mixing, model inter-comparisons and field experiments (e.g. GoAmazon model benchmark by Vila et al. 2019).

3.2.2 Lagrangian atmospheric dispersion models

Lagrangian models (LMs) track the movement of fluid parcels in their moving frame of reference (Lin et al., 2011). The most comprehensive LMs are Lagrangian Particle Dispersion Models (LPDMs) such as FLEXPART (Pisso et al. 2019) or STILT (Lin et al., 2003), which account for advective, turbulent and convective transport. LMs are known to create minimal numerical diffusion and thus are capable of preserving gradients in tracer concentration, for example in small-scale emission plumes. Additionally, Lagrangian integration is numerically stable, meaning that models can take bigger time steps. LPDMs can be run backward in time, allowing the computation of footprints (source-receptor sensitivities) as a basis for an analytical solution of the inversion problem. The downside is that LMs are computationally intensive when run for a large number of receptor points, which makes them less suited for the inversion of XCO_2 from satellites. LPDMs are offline models that run with meteorological output from both global (e.g. FLEXPART-IFS) and regional NWPs (e.g. WRF-STILT, FLEXPART-COSMO).

3.2.3 Evaluation

WP5-WP2 workshop: Transport model inter-comparison.

3.3 Biogenic fluxes

There are three main approaches to estimate prior biogenic flux information based on statistical and biogeochemical models with differing degrees of model complexity and use of observations. They all have different advantages and disadvantages which are described in sub-sections below. However, all the methods rely on accurate input data, namely:

- mapping of land use (e.g. plant functional type and vegetation cover)
- satellite observations and ancillary Earth Observation (EO) data (e.g. albedo, FAPAR, LAI, vegetation indices, vegetation activity)
- meteorological data

Errors in the input data will lead to uncertainties and even biases in the biogenic fluxes, which could impact the estimation of anthropogenic emissions. Another key source of uncertainty in current biogenic models lies in the spatialization of parameters, which is usually done by Plant Functional Type (PFT). PFT makes models sensitive to PFT maps and it is an extremely poor way of spatializing biogeochemical parameters. Data-fusion product are less dependent on the fixed PFT structures. A systematic inter-comparison and assessment of the different approaches and the evaluation of the different products with FLUXNET data can help to benchmark the different approaches (section 4.2.4). While an ensemble of products could also be useful to provide an uncertainty estimate of the prior for the atmospheric inversion.

3.3.1 Data-fusion products

Data-driven products are designed to upscale the satellite and in situ observations of biogenic fluxes (NEE, GPP) using statistical regression models and predictors from other satellite products and NWP analysis. This approach allows a direct link with observations and non-prescribed relationships between fluxes and drivers/predictors unlike process-based models.

However, it can be challenging to estimate signals on such a wide range of different timescales (e.g. from hourly to annual/decadal) which might not be well represented by the predictors in the regression leading to underestimation of the seasonal cycle (Running et al., 2004) or the inter-annual variability (Jung et al., 2019).

There are multiple types of data-fusion products:

- NEE and GPP FLUXCOM product based on machine learning methods that upscale the eddy covariance measurements (see D3.2; Tramontana et al. 2016; Jung et al., 2017; Bodesheim et al., 2018; Walther et al., 2019). Ecosystem respiration is generally taken as the residual of NEE and GPP. The main advantage of FLUXCOM is that it makes direct use of in-situ FLUXNET data; makes it is easy to use different EO data streams (e.g. SIF); it is extremely data-adaptive compared to a fixed model structure; and it facilitates the derivation of the error covariance parameterizations as it is based on the in-situ FLUXNET data. The main disadvantages are the propagation of potential biases in the in-situ FLUXNET data, and the difficulty to make it operational and include it in a full FFDAS like system.
- GPP satellite products based on statistical models using solar-induced chlorophyll fluorescence (SIF) (Joiner et al., 2018). SIF is provided by many current and future satellites (including CO2M). It is considered an important constraint for the natural fluxes and thus it would help with the attribution of the CO_2 emissions/sinks.

- GPP satellite products based on simplified light use efficiency (LUE) models (Zhang et al., 2017).

3.3.2 Simplified models

Simplified diagnostic models use empirical parameters to represent response of plants to atmospheric drivers from NWP models and satellite data, and fixed look-up tables for the empirical parameters:

- The photosynthesis models are based on light-use-efficiency models. In CHE, such simplified models include the Vegetation Photosynthesis and Respiration Model (VPRM, Mahadevan et al. 2008, see D2.3), SDBM (Knorr and Heimann, 1995), and the A-gs model (Jacobs et al, 1996, 2007; Boussetta et al., 2013).
- The ecosystem respiration component is based on an empirical formulation (Boussetta et al., 2013).
- The advantage of such empirical models is that they have few parameters that can be optimized in a CCDAS approach (e.g. Kaminski et al., 2017). Due to their simplicity and low cost, they are also suited to run at high resolution (e.g. down to 1km for VPRM simulations in CHE, see D2.3) and in NRT (e.g. Agusti-Panareda et al., 2019). Because these models are usually diagnostic and they miss complex biochemical processes, they cannot be used in climate simulations.

3.3.3 Dynamic Global Vegetation Models (DGVMs)

DGVMs are complex biogeochemical models of terrestrial vegetation that are designed to represent the mechanistic processes of enzime kinetics associated with photosynthesis (Farquhar et al, 1980) and ecosystem respiration based the representation of carbon pools (e.g. JULES, LPJ-GUESS, NCAR-CLM4, ORCHIDEE, OCN, SDVGM, VEGAS, JSBACH, BETHY).

- The advantage of these DGVM is the inclusion of many biogeochemical processes and prognostic equation of the evolution of vegetation with time. Therefore, they can be used to run simulations over climate timescales (e.g., Sitch et al., 2008).
- The limitations include the high complexity of the DGVMs (Prentice et al., 2007) which include many highly uncertain processes and parameters leading to a large spread between models (e.g. Sitch et al., 2008, 2015).

3.3.4 Evaluation

WP5-WP2 workshop:

Inter-comparison of FLUXCOM, SDBM, VPRM, A-gs (CTESSEL), ORCHIDEE, CASA-SiB, SiB4, etc with ICOS FLUXNET(2018) data in 2015 (WP2 CHE nature runs) over Europe. The caveat of this evaluation is the representation error, which could only be resolved if each model was run at the FLUXNET sites with the same observed forcing (see recommendations in section 4).

3.4 Anthropogenic emissions

Anthropogenic emissions grouped into a single source category provide a clear atmospheric signal and offer a simple option for modelling and attribution. However, a single category is no longer sufficient when considering the modelling of emissions, co-emission factors and uncertainties. Further detail can be gained by dividing emissions into sub-categories. For example, the daily temporal distribution of residential heating emissions can be modelled separately, using the heating degree day approach (e.g. Guevara *et al*., 2019a). Emissions from certain sectors (e.g. transport) are abundant in co-emitted species, which could provide additional information for sector specific attribution. The uncertainty associated with some sectors (e.g. energy) is significantly smaller than other sectors (e.g. solid waste incineration). For these reasons it is recommended that anthropogenic emissions be grouped into sectors, which can either be individually modelled and/or are representative of specific co-emitted species and specific uncertainties. The budget of each group must also be sufficiently large to generate a detectable modelled atmospheric signal, which is essential for source attribution. The following seven categories are recommended, super power stations, typical power stations, manufacturing/industry, residential combustion (settlements), aviation, non-aviation transport and other (Table 1).

3.4.1 Emission inventories based on Tier 1, Tier 2 and Tier 3 IPCC reporting

Anthropogenic emissions are typically derived with varying degrees of methodological complexity following IPCC (2006) guidelines. The estimated emissions per sector and country are the product of activity data (e.g. energy statistics) and an estimation of the quantity of emissions per unit activity (emission factor). The complexity by which the emissions are derived can be grouped into either tier-1 (basic), tier-2 (intermediate/technology-specific) or tier-3 (detailed/modelled) methodologies. Similarly, the spatial gridding of the estimated emissions can range in quality from tier-1 to tier-3 depending on the appropriateness of the spatial proxy being used for each sector, as reported by the EMEP/EEA (2016) guidelines. When comparing different emission inventories, studies sometimes show that the total amount of CO_2 emissions are quite similar but that strong discrepancies appear in their spatial distribution (e.g. allocation of CO_2 emissions related to residential heating or location of industries, Cai et al., 2018).

At a global scale the state-of-the-art emission inventory (EDGAR v4.3.2) adopts a tier-1/2 methodology; however more detailed information at the regional scale permits tier-2/3 methodologies to be adopted by European or national scale inventories (e.g. as generated by TNO in CHE WP2). The methodology adopted by the selected inventory can inform uncertainty information.

Other tier-3 regional inventories are available for the USA (Vulcan, Gurney et al. (2009), and HESTIA, Gurney et al., 2019), Canada, South America and China (e.g. CHRED, Cai et al, 2018). New tools are being developed to make use of this mosaic of regional inventories by combining them with global inventories like EDGAR at the global scale and processing them for use in atmospheric transport models (e.g. HEMCO by Keller et al., 2014 and HERMES by Guevara et al., 2019b). An example of such a merged mosaic inventory is HTAPv2.2 (Janssens-Maenhout et al., 2015). However, as inventories may differ in e.g., sector definitions, distribution proxies, etc. specific attention is needed to assure consistency across the domain.

Benchmarking:

Comparison of EDGAR and TNO inventories and links to UNFCCC over European domain and with non-European tier-3 inventories if available.

Table 1 Anthropogenic CO2 emission sectors, their global budget and co-emitters (see Table 1 from Janssen-Maenhout et al. (2019) for a description of the EDGAR sectors).

ECMWF group	EDGAR sector	IPCC2006 activity	Global budget[1]		Co-emitters		
			Total Mton	Uncertainty %	NOx	CO	PM2.5
ENERGY_S	ENE	1.A.1.a (subset)	897	-7/+2	✓	x[2]	
ENERGY_A	ENE	1.A.1.a (rest)	11'672	-7/+7	✓	X[2]	
	SWD-INC	4.C	137	-40/+40	✓	✓	✓
MANUFACTURING	IND	1.A.2	7'329	-7/+7	✓	✓	✓
	IRO	2.C.1, 2.C.2	234	-31/+31			
	NFE	2.C.3, 2.C.4, 2.C.5, 2.C.6, 2.C.7	91	-43/+72			
	NEU	2.D.1, 2.D.2, 2.D.4	25	-58/+127			
	NMM	2.A.1, 2.A.2, 2.A.3, 2.A.4	1'749	-42/+70			
	CHE	2.B.1, 2.B.2, 2.B.3, 2.B.4, 2.B.5, 2.B.6, 2.B.8	677	-50/+82			
SETTLEMENTS	RCO	1.A.4, 1.A.5.a, 1.A.5.b.i, 1.A.5.b.ii	3'323	-11/+11	x[3]	✓	✓
AVIATION	TNR-Aviation-CRS	1.A.3.a_CRS	412	-21/+70	✓	x[4]	
	TNR-Aviation-CDS	1.A.3.a_CDS	306	-14/+47	✓	x	
	TNR-Aviation-LTO	1.A.3.a_LTO	98	-12/+38	✓	x	
TRANSPORT	TRO	1.A.3.b	5'531	-4/+4	✓	✓	✓
	TNR-Ship	1.A.3.d	819	-35/+49	✓	✓	✓
	TNR-Other	1.A.3.c, 1.A.3.e	255	-29/+98	✓	✓	✓
OTHER	REF-TRF	1.A.1.b, 1.A.1.c, 1.A.5.b.iii, 1.B.1.c, 1.B.2.a.iii.4, 1.B.2.a.iii.6, 1.B.2.b.iii.3	1'918	-32/+144		✓	✓

[1] CO_2 emission budgets are based on the global emission maps used in the CHE project

[2] Power plants show high energy efficiency of the combustion at high temperature. Therefore they emit little CO but do they emit NOx. However, the de-NOx – de-SOx abatement can show high efficiencies in the range of 96-99%.

[3] Residential heating systems can vary, but if locally implemented, a boiler at home is not showing the same high temperature combustion as the power plants and so can have lower efficiency combustion with emission of CO and less NOx

[4] The turbines of airplanes are typically having a higher temperature combustion, with rather NOx emissions than CO

3.4.2 Emission vertical profiles

Local sources from power plants and industrial facilities are not emitted at surface but from chimney stacks with heights from 100 to 200m above the ground and at high temperatures their plumes can rise higher (Brunner et al., 2019). Emission vertical profiles and plume rise models are regularly used in regional air quality models (e.g. Bieser et al., 2011; Guevara et al., 2014) and they have been shown to have a significant impact on surface CO2 and XCO2 over Europe (Brunner et al., 2019). The tracer injection heights are usually computed with a plume rise model and input stack parameters like stack height, effluent temperature, and volume flux. This information is not available for the point sources over the globe and therefore some assumptions would be required to use the plume rise model on a global domain.

Emitting from a point source is not the same as emitting over a model grid cell of 10kmx10km as used currently by the IFS. Further testing of the plume rise model needs to be done to understand the impact of horizontal and vertical resolution on the most effective vertical allocation of the point source.

Benchmarking:

Impact of using sector dependent vertical profiles on atmospheric CO2 variability (e.g. Brunner et al. 2019).

3.4.3 Emission temporal profiles

Accurate modelling of anthropogenic emissions requires detailed high-resolution temporal profiles, which are often unavailable. Offline emissions are typically constant at annual (EDGAR v4.3.2, Janssen-Maenhout et al., 2019) or monthly (EDGAR v4.2FT2010) timescales. Higher temporal frequency can be included online using prescribed functions for weekly and hourly timescales (e.g. biomass burning diurnal cycle implemented in CAMS). CHE regional models apply such fixed temporal profiles over Europe (Liu et al., 2017). Global models generally do not use such high frequency profiles because it can also introduce high uncertainty, as this variability is largely dependent on country and/or climatic zones. Some generic profiles have been derived for specific regional inventories (e.g. Nassar et al., 2013, Denier van der Gon et al, 2011, Pouliot et al, 2012) and CAMS is now producing global and regional gridded temporal profiles for monthly, weekly, daily and hourly timescales for several species (e.g. NO_2, CO, PM2.5, CO_2, CH_4) and sectors based on activity data from a range of countries. For CO_2 gridded temporal profiles for energy, transport and residential heating are available. Given the high I/O requirements of using high temporal resolution emissions for the different sectors, the current strategy is to use monthly emission datasets and integrate the higher resolution temporal profiles (i.e. weekly, daily and hourly variations) in the model.

Benchmarking:

Assess impact of fixed emission temporal profiles on atmospheric CO2 variability (e.g. Liu et al. 2017).

3.4.4 Modelling fossil fuel emissions (FFDAS approach)

A fossil fuel data assimilation system offers the potential to constrain the spatial distribution of anthropogenic emissions in NRT. National statistics or nightlight observations can be used to constrain emissions based on variables such as population density, economic activity or traffic activity data. Models such as these (e.g. Rayner et al., 2010) can be used to either inform prior emissions for use in atmospheric models or they can be combined with atmospheric models and atmospheric observations of CO_2 for parameter optimisation, which can provide posterior flux information.

For certain sectors, such as residential heating, temporal profiles can be derived online using temperature values from the model atmospheric fields (e.g. Matthias et al., 2018; Guevara et al., 2019a). These can be used to update emissions at high temporal frequency. Atmospheric variables could also be used to inform energy emissions, through variability in demand. Online emissions need to be carefully configured to ensure the global budget in the model is conserved, this may require the model to be run in reanalysis mode using historical meteorological data. The advantage of this approach is that it provides a very efficient spatial and temporal disaggregation of the emission statistics.

Future developments should focus on a synergy between modelling trace gas emissions and urban schemes for numerical weather prediction (NWP). Urban schemes for NWP have varying degrees of complexity and can be considered as either slab tiles, single layer canopies or multi-layer canopies. The more basic slab (e.g. Best, 2005) and single layer canopy models (e.g. Porson *et al* 2010) could be used on a global scale using only a few parameters, which are currently available from providers (e.g. urban fraction). These produce surface temperatures, which would inform a residential emissions model. More complex emission models which require more variables may be dependent on complex multi-layer urban canopy models (e.g. Masson *et al*., 2000). Efforts have already begun to combine these local scale urban schemes with a CO_2 emission model (Goret *et al*., 2019).

Benchmarking:

Assess impact of residential heating profiles in CHE nature run on atmospheric CO_2 variability.

3.4.5 Co-emitted species and other tracers for source/sink attribution

Combustion processes, which are an important anthropogenic source for CO_2, co-emit chemically reactive species that play an important role in the chemistry of the atmosphere. Because of the rapid chemical conversions and removal processes, the spatio-temporal gradients of these species are often more pronounced than the gradients of CO_2, and they are much less influenced by biogenic activity. These two aspects make the reactive species good markers for anthropogenic emissions from different sectors (listed in Table 1). Important examples of the co-emitted species are Nitrogen Oxide (NO), Nitrogen Dioxide (NO_2), Carbon Monoxide (CO) and Sulphur Dioxide (SO_2). Most of these species are observed with the air quality in-situ network at the surface and with satellite instruments. In particular, NO_2 can be monitored at a high spatial (e.g. TROPOMI, Eskes et al., 2019) and temporal resolution (e.g. Sentinel 4) with current or planned satellite missions. Another approach for the fossil fuel attribution is to use the radioactive isotope of carbon (^{14}CO2) from in situ observations (CHE D4.1) which is depleted in fossil fuels, or Atmospheric Potential Oxygen (APO) which is based on the variation of oxygen to nitrogen ratio associated with fossil fuel combustion (see CHE D4.1 and CHE D4.3 for further details).

- CO and NOx are co-emitted by combustion processes (e.g. energy production, transport, residential heating) and therefore can provide information on attribution of specific sectors (see Table 1, CHE D4.3). We require prior information of co-emitted species in terms of emissions, atmospheric sink associated with chemistry, atmospheric initial conditions and/or emission factors (depending on the definition of the control vector in data assimilation). Emission factors depend on sector and fuel type (for CO_2) and on technology (for NOx, CO, PM2.5) and differ amongst regions and even within one country. Therefore, they are highly uncertain. The key question is whether regional spatial averages of sectoral emission factors are well characterized or whether they are chaotic (i.e. not stable) like emitter-to-emitter variations. The activity data show large temporal and spatial variability and therefore they can become highly uncertain. The initial and boundary conditions are available from the CAMS re-analysis (Inness et al., 2019).

- Radiocarbon is potentially a very useful marker to trace fossil fuel emissions. However, it is a complex tracer to model (see CHE D4.3) with limited availability of observations (CHE D5.1). This requires representation of sources (cosmogenic and nuclear power), as well as the adaptation of the atmospheric CO_2 and anthropogenic emissions (fossil fuel and bio fuels), ocean fluxes, biomass burning and biogenic CO_2 flux model in order to represent the isotope fractionation associated with all the processes (Wang, 2016; Wang et al., 2018). Initial conditions and boundary conditions for regional models are also required. In CHE they have been provided by the LMDZ simulation of Wang (2016).
- Atmospheric Potential Oxygen (APO) is also a complex tracer to model with limited availability of observations (see CHE D4.3), requiring information on: O_2 consumption flux from anthropogenic emissions (fossil fuel, biofuel); the O_2:CO_2 ratio of terrestrial biospheric exchange (per biome and soil type); gridded ocean CO_2, O_2 and N_2 fluxes; biomass burning O_2/CO_2 ratios (based on CO:CO_2 ratios); and photochemical CO and CH_4 oxidation from reaction with OH (associated with net loss of atmospheric O_2). Finally, atmospheric initial and boundary conditions are also required as input. In CHE, these have been obtained from the Jena Carboscope inversions (Rödenbeck et al, 2013).
- Carbonyl Sulfide (COS) is a tracer that can be used to constrain gross primary productivity associated with photosynthesis by vegetation (Launois et al., 2015). The observations available are described in D5.1. The model requirements comprise: atmospheric sink, its ocean emissions, its soil fluxes, its anthropogenic emissions, its biomass burning emissions and the leaf relative uptake ratio of COS to CO_2 fluxes.

3.4.6 Evaluation

WP5-WP2 workshop:

- Inter-comparison of emission data sets (e.g. EDGAR, TNO)
- Input of atmospheric modeling on the sensitivity of the used spatial distribution, the temporal profiles
- Consistency between emission fields of CO_2 and of co-emitted species
- Check on the sub-regional detailed inventory and the same region of the global inventory – the total is constrained at country level.
- Explore information in additional tracers like C14, APO.

3.5 Biomass burning emissions

Fire is an essential component of the Earth system contributing significant amounts of greenhouse gases, trace gases and particulate matter to the atmosphere. Satellite measurements of global fires provide information on the location and timing of active fires and can be used to estimate emissions using observations of either the burnt area (BA) or fire radiative power (FRP). In both cases these observations are used to estimate the dry matter consumed by fire which is used in the emission estimation based on vegetation type and emission factors derived from laboratory and field studies. Currently available datasets of fire emissions use both burned area (e.g., Global Fire Emissions Database, GFED) and FRP (e.g., Global Fire Assimilation System, GFAS; Fire INventory from NCAR, FINN). Total estimated emissions are generally consistent between the two approaches and the choice of which method to use depends on the application: the BA approach provides information on extent of burning in addition to the emissions but is not available in NRT; the FRP approach is available in NRT and is more suitable for operational applications. Improvements in estimating global fire emissions are anticipated in the near future through the use of real-time satellite observations from geostationary and LEO orbits, improvements in vegetation/land cover maps, and improved emission factors from laboratory and field studies.

3.6 Ocean fluxes

Ocean CO_2 fluxes can also be estimated using data-fusion methods with pCO_2-based products (e.g**.** Takahashi et al., 2009) or global ocean biogeochemistry models (GOBMs):

- The GOBM represent the physical, biological and chemical processes that control the CO2 concentration in the ocean (e.g. CCSM-BEC, Doney et al. (2009); MICOM-HAMOCC, Schwinger et al., 2016; MITgcm-RecoM2, Hauck et al., 2016; MPIOM-HAMOCC, Mauritsen et al., 2019; NEMO-PISCES (CNRM), Berthet et al., 2019; NEMO-PISCES (IPSL), Aumont and Bopp, 2006; NEMO-PlankTOM5, Buitenhuis et al., 2010). Like the DGVMs they require inputs for the atmospheric forcing (e.g. from NWP re-analysis). They are complex costly models, with prognostic skill to run in climate simulations.
- Data-based products are designed to exploit all the available pCO_2 observations over the ocean from the SOCAT database using either neural networks (e.g. Landschützer et al.,2015) or simple parameterizations of the ocean mixed layer (e.g. Rödenbeck et al., 2014).

A comparison between the annual ocean CO_2 sink from GOBM and pCO_2 flux products shows there is consistency in the underlying variability (Le Quéré et al., 2018).

3.7 Atmospheric chemistry

Modelling combustion short-lived species (CO and NO_x) to infer CO_2 sources requires the simulation of the chemical conversions, removal processes and the emissions in the atmosphere. Of particular importance are the fast chemical conversions between the emitted but very-short lived NO and the longer lived but well-observed NO_2 in the presence of other chemical species such as ozone and OH. Chemical schemes comprising of 50-120 species have been integrated in the IFS as part of the GEMS, MACC and CAMS projects (Flemming et al, 2015, Huijnen, et al. 2019). The IFS in CAMS configuration is used operationally to forecast atmospheric composition and to assimilate satellite retrievals of NO_2, CO, ozone, SO_2 and Aerosol Optical Depth (Inness et al. 2019).

But, the computational cost of the chemical schemes is considerable, which may require the development of computationally affordable but still adequate versions of the chemistry scheme for the application in CHE. The development of simplified schemes is already a growing research focus in CAMS because affordable schemes are intended to be used to better represent atmospheric chemistry in the tangent-linear and adjoint formulation of the IFS applied in the 4DVAR data assimilation approach. For example, the development of a surrogate model for chemistry using machine learning algorithms will be developed as part of a NASA project run by University of Colorado in collaboration with ECMWF.

4 Recommendations for operational CHE prototype

Table 2: Implementation 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.

Topic identifier	Component	Domain	Stream	Recommendation	Estimated effort (Person Months)
IM-TRA-1	Transport	global regional	NRT RA	Implement and test near mass-conserving advection scheme in online models (e.g. COMAD semi-Lagrangian and MPDATA advection schemes in the IFS)	12 to 36 months
IM-TRA-2	Transport	global regional local	NRT RA	Evaluation of turbulent mixing and convective transport using Radon and other tracers (vertical gradients)	12 months
IM-TRA-3	Transport	global regional	NRT RA	Inter-comparison of global, regional and local models to evaluate local transport by plumes.	12 months
IM-AEM-1	Anthropogenic emissions	Local (Point Sources)	RA	Characterisation of emission source with all parameters and have plume model for each or for a group of them (evaluate how to group these into "clumps")	12 to 36 months
IM-AEM-2	Anthropogenic emissions	Global	NRT RA	Introduce online fixed spatio-temporal profiles for different sectors at weekly, daily, hourly scales (e.g.	12 months

				Guevara et al. 2019, Nassar et al. 2013).	
IM-AEM-3	Anthropogenic emissions	Global Regional	NRT RA	Vertical profiles of emissions (e.g. Brunner et al. 2019) (emission heights + temperature-dependent injection velocities)	12 months
IM-AEM-4	Anthropogenic emissions	Global Regional	NRT	Modelled temporal profiles with meteo predictors (e.g. residential heating) to support FFDAS approach.	12 months
IM-BIO-1	Biogenic fluxes	Global Regional Local	RA	Extensive site-level cross-validation model intercomparison excercise where models are run at site-level with site-level measured meteo (and high res satellite data cutouts if needed). This would be really helpful and insightful to judge on the qualities and gaps between GPP and NEE models of different kind and complexity. It would also open doors for estimating the spatial-temporal errors and error covariance parameterisations for the different models.	36 months
IM-BIO-2	Biogenic fluxes	Global Regional	NRT	Test improved high resolution mapping of land use in models: classification, cover, including vegetation mapping (CGLS, Buchhorn et al.,2017; ESA-CCI, 2017; ECOCLIMAP Champeaux et al, 2005; GLCC,	24 to 36 months

				Loveland et al., 2000; urban settlement dataset from JRC, Pesaresi et all, 2016)	
IM-BIO-3	Biogenic fluxes	Global Regional	RA	Improve simplified model to use information on SIF and COS	36 months
IM-BIO-4	Biogenic fluxes	Global Regional	RA	Test impact of land use change with simplified, data-driven and DGVM	36 months
IM-BIO-5	Biogenic fluxes	Global Regional	RA	Inter-comparison of DGVM, simplified and data-fusion models (multi-model ensemble to characterise uncertainty)	12 to 24 months
IM-CHM-1	Chemistry	Global Regional	NRT RA	Develop computationally affordable chemistry for co-emitted tracers (NO_2, CO, PM2.5, NMVOC)	36 months

5 Research priorities

Table 3: 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.

Topic identifier	Component	Domain	Stream	Recommendation	Estimated effort (Person Months)
RS-TRA-1	Transport	Global Regional	NRT RA	Test new transport schemes developed in NWP, e.g. MPDATA advection in FVM IFS	36 months

				(Kühnline et al, 2019)	
R-TRA-2	Transport	Global Regional Local	NRT RA	Integrate plume rise model in emission hotspots (Guevara et al, 2014, Brunner et al., 2019)	24 months
RS-TRA-3	Transport	Regional Local	NRT RA	Evaluate PBL wind profiles crucial for plume modelling (Sandu et al., 2013)	12 months
RS-AEM-1	Anthropogenic emissions	Global Regional Local	NRT RA	Extend FFDAS approach using all available human activity proxies.	24 months
RS-AEM-2	Anthropogenic emissions	Global	RA	Merge mosaic of regional inventories (Tier 2,3) with global inventory (Tier1, Tier2).	12 months
RS-BIO-1	Biogenic fluxes	Global Regional	NRT RA	Use SIF and COS to constrain biogenic fluxes	24 to 36 months
RS-BIO-2	Biogenic fluxes	Global Regional	RA	Introduce crop modelling and relevant land management information (crop rotation/harvesting, grazing, etc.)	24 to 36 months
RS-TRC-1	Other tracers	Regional		Implementation of APO and radiocarbon in forward/inverse model.	36 months

6 Conclusion

This report presents the options for a high-resolution modelling and prior flux estimation capability in the context of the CHE CO_2 prototype based on: multi-scale (global, regional and local) and multi-stream (NRT and re-analysis) models and products. These options will be refined in the final report. The outcome of the WP2-WP5 workshop on model evaluation will provide further guidance by addressing the following aspects:

- Inter-comparison of global, regional and local models used in the various CHE nature runs (CHE D2.1, CHE D2.2).
- Inter-comparison of different GPP and NEE products and models in the CHE nature runs (CHE D2.3 and CHE D3.2).
- Case studies of plumes from hotspots with different transport models.

7 Acronyms

Table 4 List of acronyms

APO	*Atmospheric Potential Oxygen*
CAMS	*Copernicus Atmosphere Monitoring Service*
CASA	*Carnegie-Ames-Stanford Approach*
CFL	*Courant–Friedrichs–Lewy or CFL condition*
CNRM	Centre National de Recherches Météorologiques
COSMO	*Consortium for Small-scale Modeling*
CTM	*Chemical Transport Model*
DGVM	*Dynamic Global Vegetation Model*
ECMWF	*European Centre for Medium Range Weather Forecasts*
EDGAR	*Emissions Database for Global Atmospheric Research*
EEA	*European Environmental Agency*
EMEP	*European Monitoring and Evaluation Programme*
EO	*Earth Observation*
ESA-CCI	*European Space Agency – Climate Change Initiative*
ESM	*Earth System Model*
FAPAR	*Fraction of Absorbed Photosynthetically Active Radiation*
GLCC	*Global Land Cover Characterization*
GOBM	*Global Ocean Biogeochemistry Models*
GPP	*Gross Primary Production*
ICOS	*Integrated Carbon Observation System*
IFS	*Integrated Forecasting System*
IEA	*International Energy Agency*
IPCC	*The Intergovernmental Panel on Climate Change*
IPSL	*Institut Pierre Simon Laplace*
LAI	*Leaf Area Index*
LEO	*Low Earth Orbit*
LM	*Lagrangian model*
LMDz	*Laboratoire de Météorologie Dynamique (LMDz) GCM*
LPDM	*Lagrangian Particle Dispersion Models*
LUE	*Light Use Efficiency*
NASA	*National Aeronautics and Space Administration*
NCAR	*National Center for Atmospheric Research*

NEE	*Net Ecosystem Exchange*
NRT	*Near Real Time*
NWP	Numerical Weather Prediction
ORCHIDEE	*Organising Carbon and Hydrology In Dynamic Ecosystems*
PFT	*Plant Functional Type*
RESP	*Ecosystem Respiration*
SiB	*Simple Biosphere*
SIF	*Solar Induced Fluorescence*
SDBM	*Simple Diagnostic Biosphere Model*
SOCAT	*Surface Ocean CO_2 ATlas*
UNFCCC	*United Nations Framework Convention on Climate Change*
VPRM	*Vegetation Photosynthesis and Respiration Model*
WRF	*Weather Research and Forecasting*

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Document History

Version	Author(s)	Date	Changes
0.1	Anna Agusti-Panareda et al.	25/11/2019	First draft shared with CHE consortium
0.2	Anna Agusti-Panareda, Dominik Brunner et al.	6/12/2019	Input of WP leaders and CHE consortium
0.3	Anna Agusti-Panareda, Dominik Brunner et al.	9/12/2019	Internal review
1.0	Anna Agusti-Panareda, Dominik Brunner et al.	19/12/2019	Revised report with feedback from reviewers (R. Munro and A. Webb)

Internal Review History

Internal Reviewers	Date	Comments
R. Munro (EUMETSAT)	13/12/2019	Positive review with recommendations to check acronyms and introduce identifiers for the individual recommendations
Webb (U. Leicester)	17/12/2019	Positive review with no specific requests.

Estimated Effort Contribution per Partner

Partner	Effort
ECMWF	4
EMPA	1.0
JRC	0.5
TNO	0.25
MPI-BGC	0.25
LSCE	0.25
iLab	0.25
WU	0.25
ULUND	0.25
Total	**7**