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Horizon 2020 Societal challenge 5: Climate action, environment, resource efficiency and raw materials

VERIFY

Observation-based system for monitoring and verification of greenhouse gases

GA number 776810, RIA

Deliverable number (relative in WP)	**D2.9**
Deliverable name:	Uncertainty analysis for the dynamical inventory model
WP / WP number:	WP2
Delivery due date:	M18
Actual date of submission:	M18
Dissemination level:	Public
Lead beneficiary:	WU
Responsible scientist/administrator:	W. Peters (WU)
Contributor(s):	I. Super (WU/TNO)
Internal reviewer:	/

1. Changes with respect to the DoA

It was agreed with the users of the uncertainty data that the actual product will be adapted to their specific needs. Therefore, this report describes the applied methodology and shows an example of the output.

2. Dissemination and uptake

(Who will/could use this deliverable, within the project or outside the project?)

The goal of this deliverable is to support inverse modelling efforts within Verify, by providing important information for determining the optimization strategy and by providing a full covariance of uncertainties in the anthropogenic emissions. This information will be used in tasks 2.3.3 and 2.4. It will be also useful in WP3 for the atmospheric inversion of the natural CO_2 fluxes, providing uncertainties for the fossil fuel emissions that are prescribed. Furthermore, this deliverable could support the synthesis in WP5 by providing uncertainties in bottom-up inventories.

3. Short Summary of results (<250 words)

This report describes a statistically coherent methodology to establish uncertainties in gridded emission inventories/models. Uncertainties in the underlying parameters (activity data, emission factors, spatial proxy maps and time profiles) are established and used in a Monte Carlo simulation to determine how they affect the uncertainty in the total emissions. This can be done at different levels of detail, e.g. per country or source sector, but also at different spatiotemporal scales. The results are shown to be useful for inverse modelers for several reasons:

- It gives insight in which model parameters are most important and should (at least) be optimized
- It provides a covariance matrix of uncertainties at the required level of detail
- It can be used to characterize the temporal/spatial correlation lengths of the uncertainties in the emissions

4. Evidence of accomplishment

(report, manuscript, web-link, other)

The results of this work are disseminated to all VERIFY partners and accessible under a SharePoint platform. Note also that part of this work was done as a PhD project and is published in a dissertation (Super, 2018).

Version	Date	Description	Author (Organisation)
V0	20/6/2019	Creation/Writing	I. Super (TNO)
V1	11/7/2019	Writing/Formatting/Delivery	I.Super (TNO) W. Peters (WU)
V2	13/8/2019	Formatting/Delivery on the Participant Portal	H. Denier van der Gon (TNO) Stephanie Kirschke (Arttic)

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1. Introduction

Atmospheric CO_2 inverse modelling studies often aim to better constrain CO_2 emissions as a whole. However, there is an increasing demand to understand changes in CO_2 fluxes in more detail, for example to identify the impact of specific emission reduction policies. Moreover, inverse modelling is done at an increasingly higher spatiotemporal resolution. One of the main challenges related to this higher level of detail and resolution in inverse modelling is the characterization of the covariance matrix of the uncertainties in the emission inventories that the inversion, in theory, corrects. Although the uncertainty in annual CO_2 emissions are relatively well-known, it is unclear how much the uncertainty increases due to spatiotemporal disaggregation.

Both the dynamic emission model developed at WU in collaboration with TNO and described in VERIFY MS9 (Testing of the ffCO2 emission model (FFDAS) for one source sector) and 'regular' emission inventories use all kinds of (statistical) data to calculate emissions per sector and region. The uncertainty in these activity data can be estimated and be used to calculate the uncertainty in the emissions. This report discusses the methodology used to determine uncertainties in emissions (also per sector) and how this supports inverse modelling efforts. We use examples from both a regular emission inventory (see D2.1) and the dynamic emission model, using the same approach.

2. Methodology

2.1. Emission and uncertainty data

Generally, gridded emissions per source sector are calculated in three steps:

1) The annual emission per country: calculated from activity data and emission factors
2) Collection of available (direct) spatially distributed emissions for example from point source databases
3) Spatial downscaling of remaining national scale (diffuse) emissions using proxy maps
4) Temporal downscaling using time profiles

Both the dynamic emission model(used for data assimilation and emission prediction) and a regular emission inventory e.g. as described in VERIFY D2.1 and subsequent updates use this approach, although different sources of data are used to calculate emissions and their uncertainties. This is described in more detail below.

2.1.1. The dynamic emission model

The dynamic emission model has only been applied to the Netherlands so far. The activity data are based on national energy statistics and are assumed to be well-known (no uncertainty). The emission factors are gathered from large databases, for example from the IPCC and EEA. These databases give a range of possible values per source sector, often even further disaggregated

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per fuel type. The median value is taken as starting point for the emission calculation and is not necessarily representative for a country. Although better estimates are available for the Netherlands, this approach was used to illustrate the application for data-poor regions. The given emission factor range also gives us the uncertainty, which is in some cases affected by necessary assumptions (e.g. on the fuel type or car fleet composition). For the CO_2 co-emitted species CO and NO_x emission factors the uncertainty is often lognormal, which is taken into consideration in the Monte Carlo simulation.

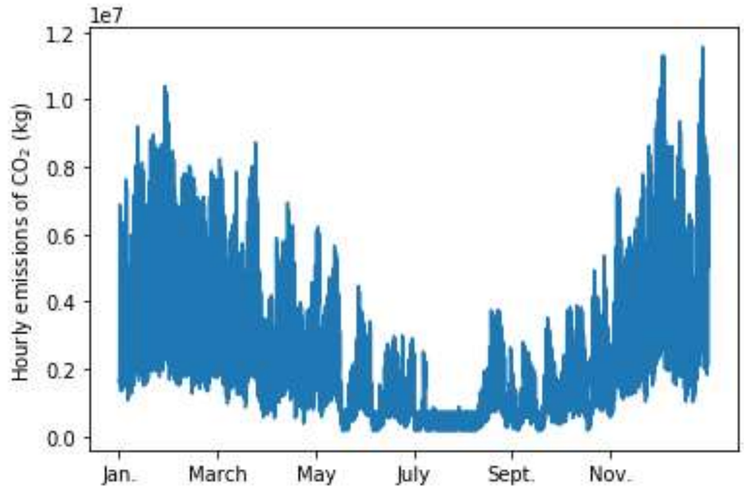

Figure 1. Hourly emissions of residential heating (households) for the Netherlands.

We then use the generic time profiles delivered with the regular TNO emission inventory (Denier van der Gon et al, 2011) and compare them to dynamic profiles based on hourly activity data (Super, 2018) to establish the uncertainty in these time profiles. An example of such dynamic emissions is shown in Figure 1.

For more details on uncertainties in the dynamic emission model, please see milestone MS31. MS31 describes a draft uncertainty framework using a fossil fuel emission model developed to calculate emissions of CO2 and co-emitted species at high resolution from statistical parameters. The draft uncertainty framework gives insight in how the uncertainty in a range of parameters translate into uncertainties in the emissions of CO2 and co-emitted species (CO/NOx).

2.1.2. The regular emission inventory

The regular emission inventory starts from collecting country-level reported emissions at very detailed level (NFR (nomenclature for reporting) sector – fuel combinations). Note that this is different from the dynamic emission model which calculates emissions “bottom-up” from activity data and emissions factors. The uncertainties were defined separately for activity data and emission factors and combined using the standard formula for error propagation for non-correlated normally distributed variables. Also uncertainties in spatial and temporal variations were considered. For example, if we have exact point source coordinates, the uncertainty in the spatial distribution is zero but if we use a proxy like industrial area land use the uncertainty can be substantial because we do not know exactly what type of facilities are located on which parts

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of the industrial land use map. Moreover, the emission inventory spans a much larger (European) area, not just one country (see Figure 2 for an example).

Uncertainties in activity data are taken from the National Inventory Reports, similar to the CO_2 emissions themselves. They are also defined per NFR sector – fuel combination and averaged for all countries (variations between countries are small). The uncertainties in CO_2 emission factors are acquired in the same way. CO emission factor uncertainties are taken from the EEA Guidebook (EEA, 2016), supplemented by BREFs (Best Available Techniques (BAT) reference documents, https://eippcb.jrc.ec.europa.eu/reference/) because CO is an air pollutant and not included in the NIR or UNFCCC and IPCC guidelines. For NOx a similar approach should be followed but this is not yet done as the first request was for a CO2 / CO dataset. Often the CO emission factor uncertainties have a lognormal distribution.

In contrast to the dynamic emission model, the uncertainties in spatial proxies are also taken into account here. They are based on expert judgement, separately for each NFR sector – proxy map combination, and often have a lognormal distribution. As mentioned before, the uncertainty in the spatial distribution of large point sources is assumed to be negligible. The uncertainties in time profiles are determined in the same way as for the dynamic emission model, using hourly activity data from different years/locations to take into account the full range of possibilities.

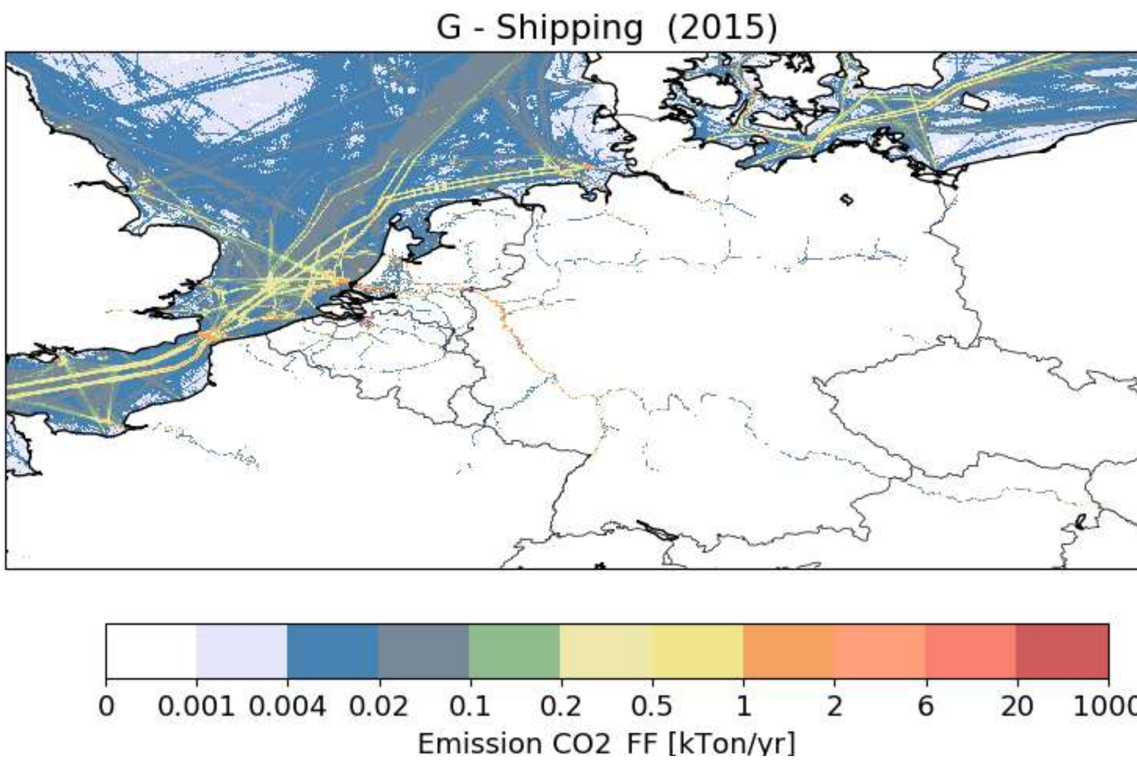

Figure 2. CO_2 emission from fossil fuel combustion in shipping.

It is important to realize that the uncertainty of some parameters can be correlated. This means that if for these parameters, something is adjusted, also the correlated parameters will be

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adjusted. For example the uncertainty in the emission factors of gasoline for passenger cars and light duty vehicles because they both use the same fuel.

2.2. The Monte Carlo simulation

The proposed methodology to translate parameter uncertainties into emission uncertainties is a Monte Carlo simulation. In a Monte Carlo simulation random samples are drawn from the parameter distributions, which are used to calculate the emissions. This results in a range of possible emissions, reflecting the uncertainty in the underlying parameters. A Monte Carlo simulation can give output at different levels, for example per country or per aggregated sector, which helps diagnosing the patterns of uncertainties and to understand which factors dominate of the overall uncertainties.
In case of the dynamic emission model the Monte Carlo simulation is relatively simple, given the small number of parameters (M = 42) and that uncertainties in spatial proxies are not considered. Therefore, a large ensemble is used (N = 500). However, for the regular inventory a much smaller sample is taken (N = 10). Here, a total of 112 subsectors (including fuel disaggregation) is included for 2 species (M = 224). Moreover, the spatial proxy uncertainty is included for a total of 59 subsectors (fuels are aggregated, because they have the same spatial distribution). Therefore, this Monte Carlo simulation results in 10 different emission maps for CO_2 and CO per GNFR sector (aggregated NFR sectors). The whole processes is illustrated in Figure 3.

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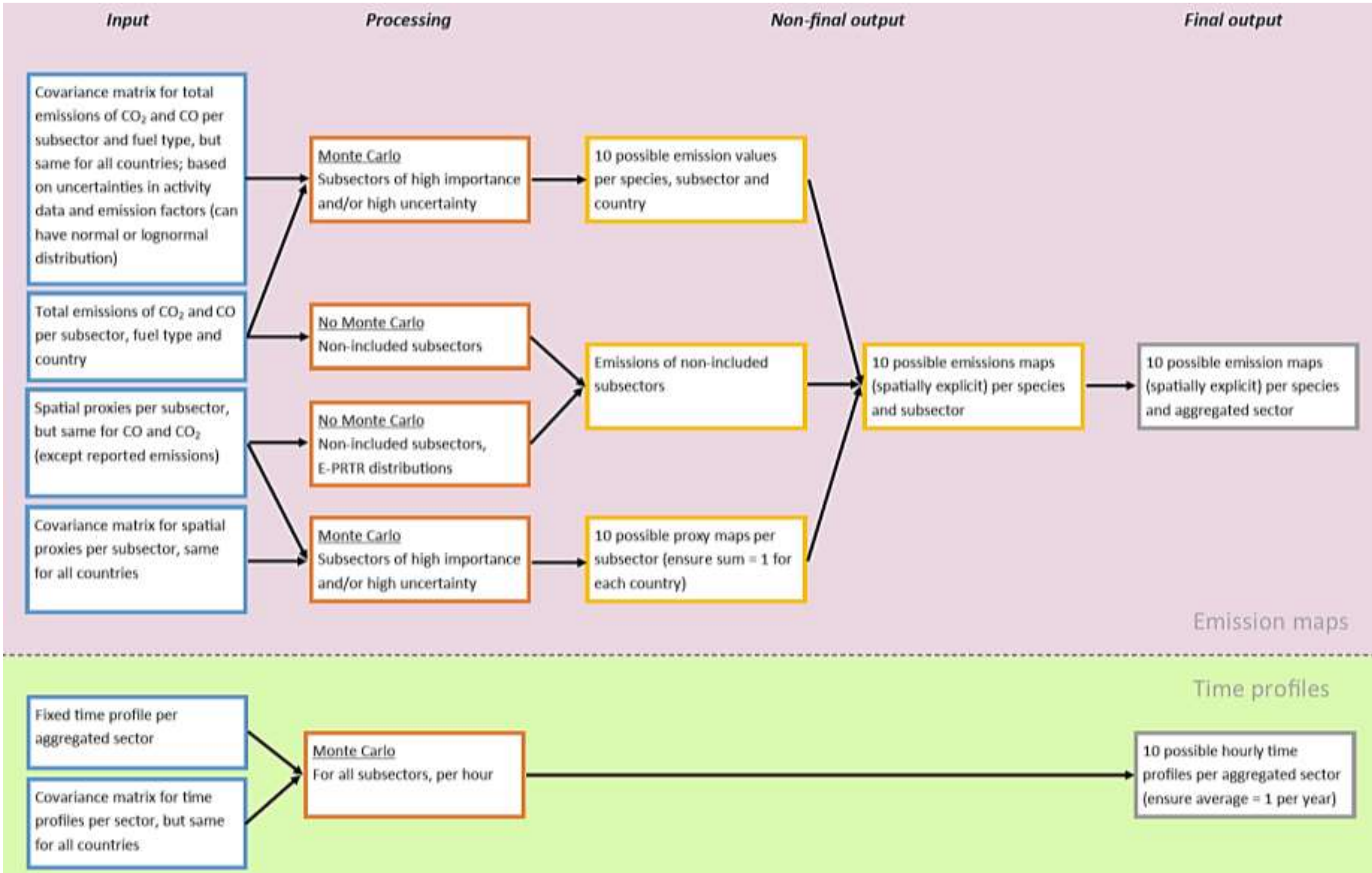

Figure 3. Flow diagram showing the input, processing and output of the Monte Carlo simulation for the regular emission inventory.

3. Results

3.1. Uncertainties per GNFR sector

From the Monte Carlo simulations with the regular annual emission inventory at 01 x 0.05 lat-lon for the year 2015(delivered in deliverable D2.1) we get the uncertainty per GNFR source sector. Figure 4 shows the normalized spread in emissions per sector for the whole domain, but this can also be split by country. For most sectors the range for CO_2 emissions is only a few %. Moreover, the largest uncertainties (e.g. fugitives and road transport – LPG gas) are for relatively small sectors (see Table 1). In contrast, public power contributes 33% to the overall CO_2 emissions, but has a relatively small uncertainty.

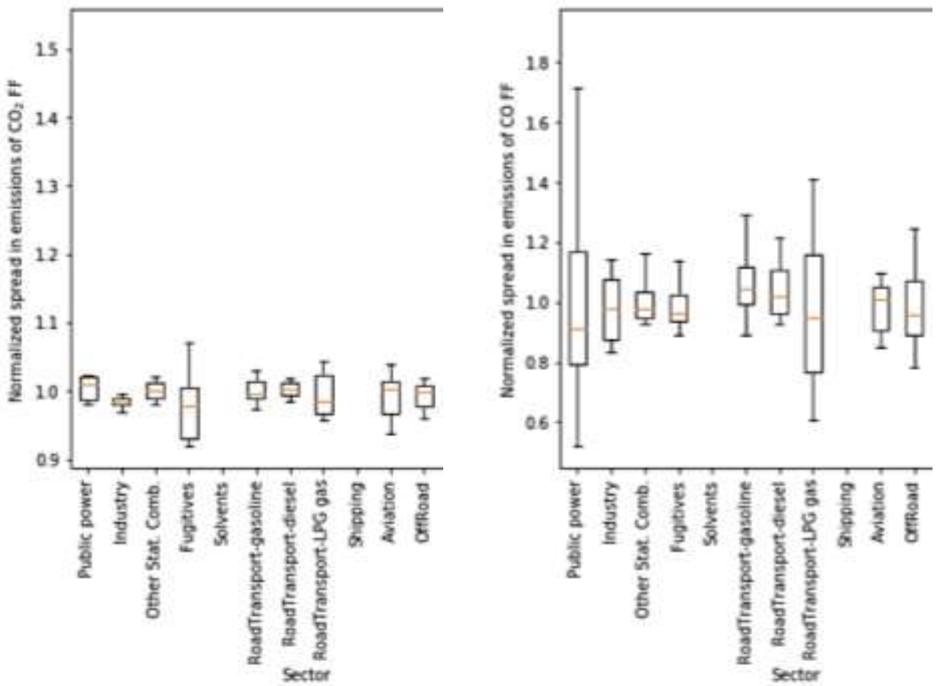

Figure 4. Normalized spread in emissions per source sector for CO_2 (left) and CO (right); Note the different scales of the Y-axis in both figures.

For CO the spread is much larger and there are some high outliers due to the lognormal shape of the uncertainties in CO emission factors. Note that the uncertainty in the spatial proxies does not affect the total emissions, only the spatial distribution.

Table 1. Mean (CO_2) or median (CO) and upper/lower limits of emissions per source sector based on the Monte Carlo simulation.

GNFR sector	CO_2 emissions (kg/yr)	CO emissions (kg/yr)
Public power	5.88E11 (5.74E11 – 5.99E11)	2.11E8 (2.05E8 – 2.16E8)
Industry	4.01E11 (3.98E11 – 4.05E11)	4.17E9 (3.43E9 – 5.26E9)
Other stat. combustion	3.17E11 (3.10E11 – 3.27E11)	7.95E8 (7.34E8 – 9.22E8)
Fugitives	2.48E10 (2.32E10 – 2.70E10)	2.14E7 (1.97E7 – 2.57E7)
RoadTransport-gasoline	1.24E11 (1.21E11 – 1.28E11)	6.12E8 (5.22E8 – 7.57E8)
RoadTransport-diesel	2.95E11 (2.989E11 – 3.06E11)	1.37E8 (1.24E8 – 1.63E8)
RoadTransport-LPG gas	5.31E9 (5.312E9 – 5.58E9)	2.73E7 (1.75E7 – 4.06E7)
Aviation	8.34E9 (7.88E9 – 8.73E9)	4.24E7 (3.57E7 – 4.61E7)
OffRoad	2.81E10 (2.72E10 – 2.88E10)	7.56E8 (6.19E8 – 9.82E8)

Figure 5 shows gridded CO emissions for the off-road sector for 2 ensemble members. Note the different ranges on the color bars. The second ensemble member apparently has some large emissions. However, for example, the emissions in the UK are overall slightly lower. This is because the Monte Carlo is performed separately for each country, so that one country can have a lower emission and another country can have a higher emission than average in the same ensemble member. With these emission maps a spatial correlation length can be determined for the covariance structure used in inversions.

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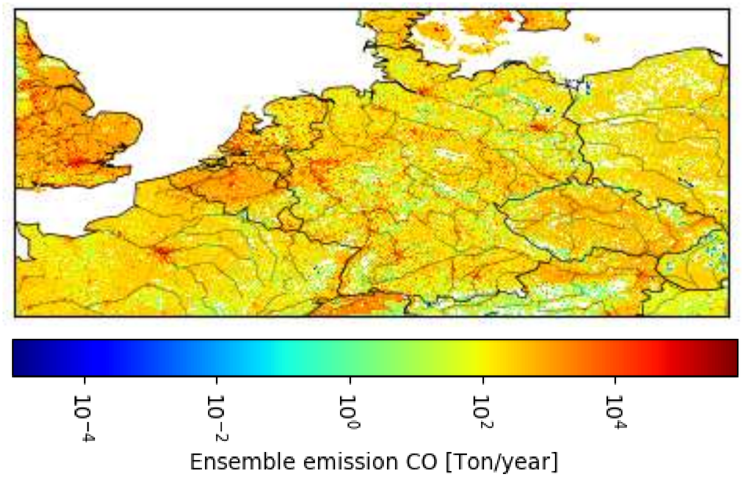

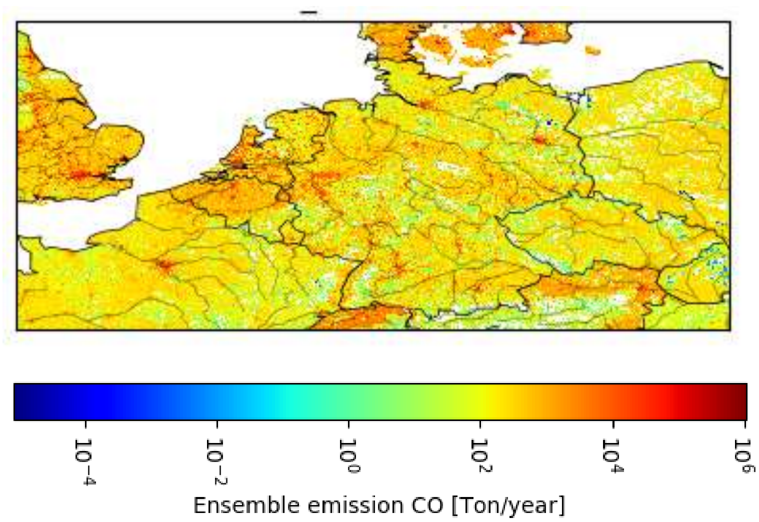

Figure 5. Gridded CO emissions for the off-road sector for 2 different ensemble members.

3.2. Importance of parameters

Using the Monte Carlo simulation with the dynamic emission model we can show how large the impact of each individual parameter uncertainty is on the overall uncertainty in the total/sectoral emissions. The effect of a parameter uncertainty on the total emission uncertainty depends on its own value, but also on the importance of the parameter in calculating the total emissions. For example, shipping only makes up a small fraction of the total CO_2 emissions. Therefore, parameters related to shipping are relatively unimportant for the uncertainty in the total CO_2 emissions.

We can examine the importance of individual parameters by performing a Monte Carlo simulation per parameter, setting all other parameters to the expected value. The result for CO_2 is shown in Figure 6. We find that the largest uncertainty is caused by the emissions factors of power plants (EF 1A) and industry (EF 3), which are the two largest sources of CO_2. This kind of analysis can help to select the parameters to be optimized in an inversion, which would be the most uncertain/important ones.

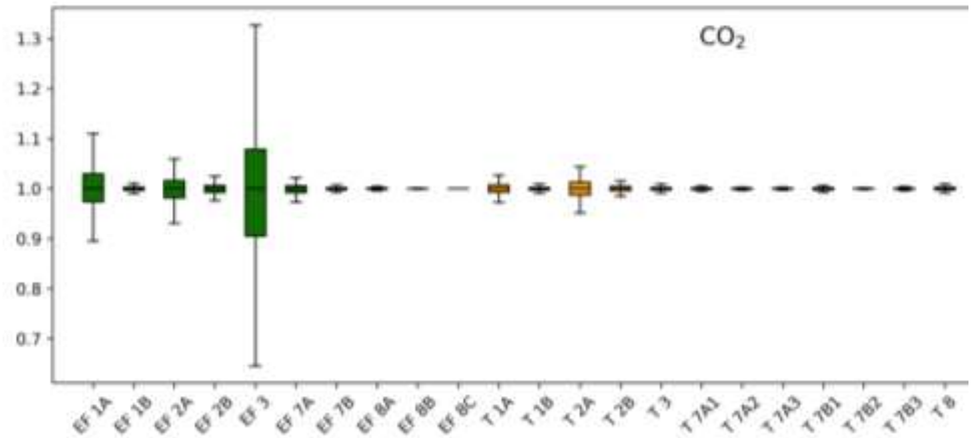

Figure 6. Normalized spread in total CO_2 emissions caused by the uncertainty in individual parameters. Shown here are emission factors (EF) and time profiles (T) per (sub)sector (in IPCC / UNFCCC sector coding).

4. Outlook

The methodology described in this report can be generally applied to each emission inventory that uses (statistical) data.

Previously, uncertainties in high-resolution gridded emissions were mostly estimated from a comparison of different emission maps. Here, we described a methodology that is supported by data and can be documented more easily. However, the required covariance of uncertainties depends on the set-up of the inversion, e.g. its spatiotemporal resolution and whether it optimizes emission model parameters or just the total emissions (per sector). As is shown in this report, uncertainties can be delivered at different levels of detail. Therefore, we included no dataset with the deliverable and instead will deliver a dataset to the inverse modelers in Verify directly after discussing their needs. Two scientific papers describing the emission model and the uncertainty framework are in preparation (one submitted in august 2019) and will be submitted in 2019. These papers will provide a reference for the inversion framework by giving a detailed description of the methodology.

While the methodology is generally applicable and reproducible, preparing the data to be used in the framework (e.g. uncertainties in individual emission factors) is a time consuming effort and partly relies on expert estimates. Therefore, producing a similar dataset for other co-emitted species than CO is feasible but ample time to make it should be reserved.

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