Atmospheric inverse modelling for estimating national-scale GHG emissions:

Current state-of-play and the need for a best practice

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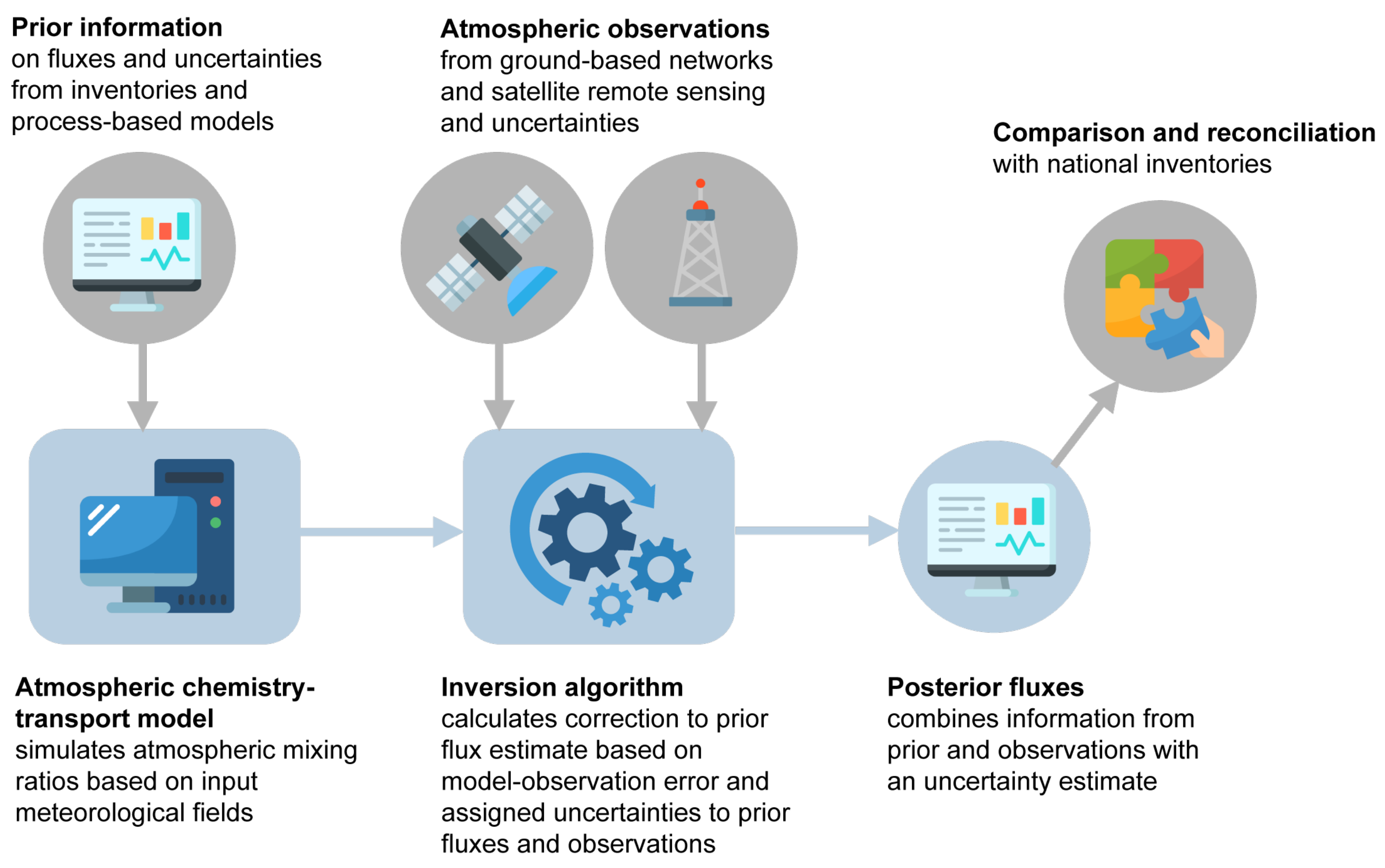
Atmospheric inverse modelling

Atmospheric inverse modelling is a method for estimating greenhouse gases (GHG) fluxes based on atmospheric observations and is being increasingly used to assess and improve inventories of emissions at national scales. It is referred to in the 2006 (and 2019) IPCC Guidelines on national reporting as a way to independently verify national emission inventories. However, the method is technically complex and can be prone to large uncertainties, especially when it is not well implemented.

Figure 1. Schematic of atmospheric inverse modelling



Prior information
on fluxes and uncertainties from inventories and process-based models

Atmospheric observations
from ground-based networks and satellite remote sensing and uncertainties

Comparison and reconciliation
with national inventories

Atmospheric chemistry-transport model
simulates atmospheric mixing ratios based on input meteorological fields

Inversion algorithm
calculates correction to prior flux estimate based on model-observation error and assigned uncertainties to prior fluxes and observations

Posterior fluxes
combines information from prior and observations with an uncertainty estimate

Current state-of-play

Different countries and even institutes have their own atmospheric transport models and inverse modelling frameworks. Differences between these and their implementation - and the current lack of metrics and quality control for inversion results - will jeopardise confidence in this method of emissions verification. Frameworks can be broadly grouped into two types: global and regional.

Global inversion frameworks

Advantages: Global coverage thus giving global mass balance and equal treatment of all regions. Current resolution order of 2 to 3 degrees but state-of-the-art systems moving to order of 1 degree resolution with massive parallelisation.

Disadvantages: Still relatively coarse compared to regional inversions and often do not incorporate regional observation networks.

Regional inversion frameworks

Advantages: Higher resolution compared to global frameworks, order of 0.5 to 0.1 degrees and often incorporate regional observation networks.

Disadvantages: Results depend on uncertain boundary conditions and no direct constraint of global mass balance.

Main sources of uncertainty

The accuracy of the posterior fluxes is compromised by the following main causes:

- **Modelled transport and chemistry errors**
  Transport errors are non-random and can be due to: i) finite resolution of the model and input meteorological data, ii) errors in physical parameterisations, iii) errors in input meteorological data, iv) inappropriate representation of site (e.g. grid cell chosen to represent site in model, Figure 2). Chemistry errors concern inaccurate estimates of atmospheric production or loss of the species of interest (e.g. OH oxidation of CH_4, or CO_2 production from oxidation of CO).
- **Poorly assigned uncertainties**
  Underestimation of uncertainty in observation space (i.e. uncertainty of the measurement and model representation) can lead to errors in the posterior fluxes; large model-observation differences have a strong impact on the posterior solution, however if this is due to the model or measurements, this will result in errors in the fluxes. Conversely, overestimation of observation space uncertainty (or underestimate of prior flux uncertainty) will limit the gain in information from the observations.
- **Dependence on boundary conditions**
  Boundary conditions include e.g. the initial mixing ratios used in the transport model and, for regional inversions, the mixing ratios at the temporal and spatial limits of the regional model (which determine the so-called "background mixing ratio"). The boundary conditions may be optimized in addition to the fluxes. Errors in the boundary conditions (especially if these are not optimized) will lead to errors in the prior fluxes. An overestimate of the background mixing ratio will lead to an underestimate of the fluxes and vice-versa (Figure 3).
- **Dependence on prior information**
  Posterior fluxes are not independent from the prior estimates. This dependence is determined by the prior and observation space uncertainties, number of observations and their information content. Posterior fluxes from inversions using different prior estimates are, therefore, not directly comparable, and if they are to be compared they need to be adjusted for the different prior fluxes.

Figure 2. Annual mean CH_4 fluxes with spuriously low fluxes around mountain sites (white circles) due to their misrepresentation in the transport model.

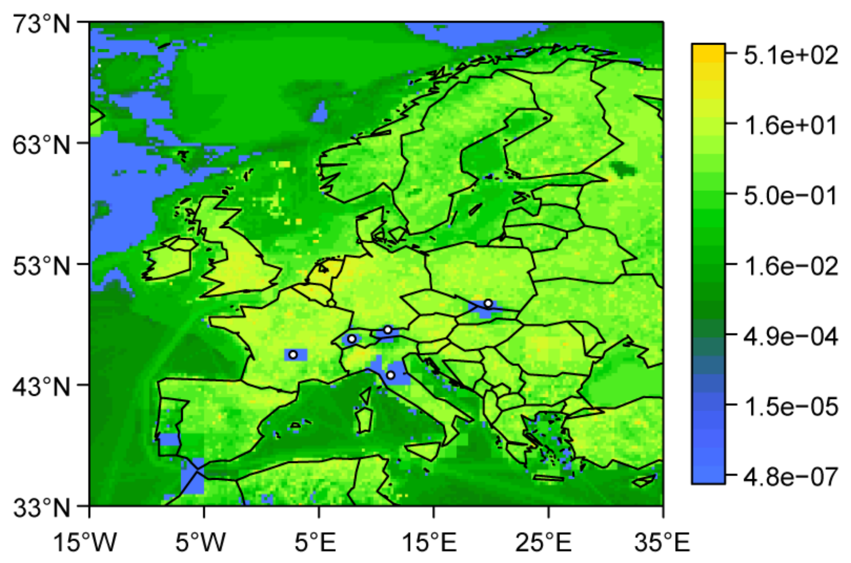
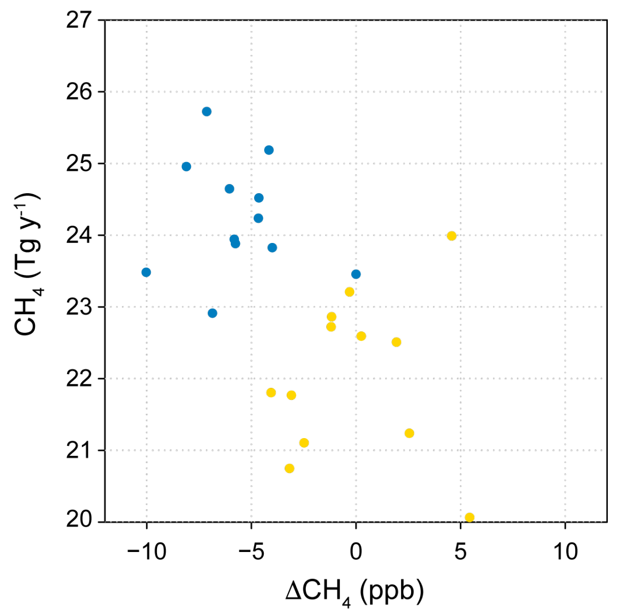


Figure 3. Dependence of the annual CH_4 source (for EU27+UK) on background mixing ratio error. Real data from two regional inversions of 12 years.



Outline of a best practice

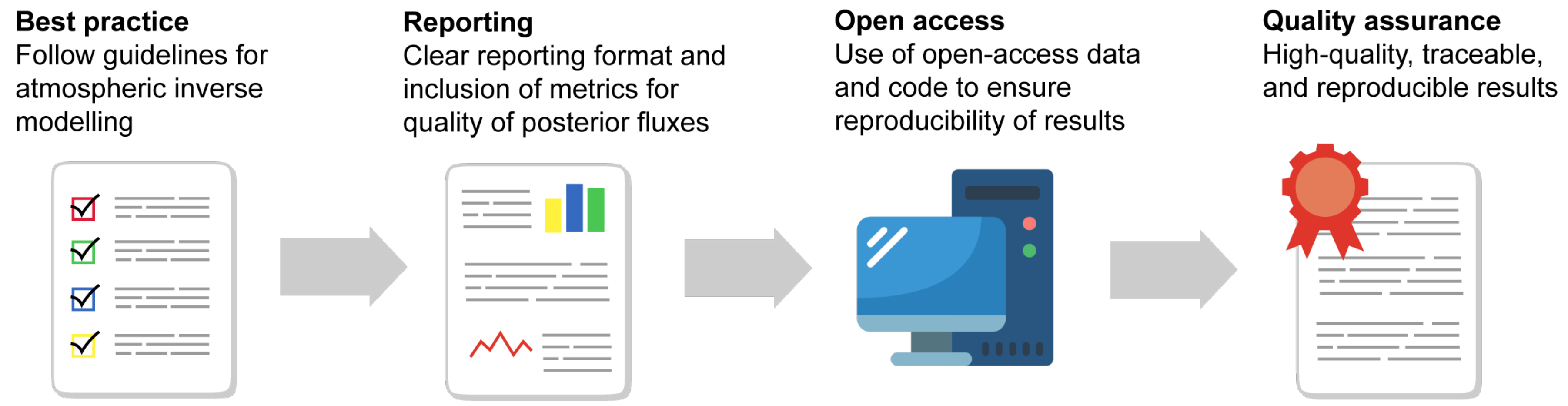
Best practice in atmospheric inverse modelling

- **Atmospheric transport model:** previously assessed, sound-basis in scientific literature, appropriate to the study (inclusion of relevant chemistry, domain and resolution).
- **Domain and resolution:** domain large enough to be able to provide a regional estimate that can be compared with independent estimates and resolution appropriate for modelling observations and for determining national estimates.
- **Atmospheric observations:** inter-comparability with other networks, quality assured, open-access, data selection appropriate to transport model, and correct representation in the model (for ground-based sites, e.g. choosing location/grid cell that best represents each site, and for satellite data, e.g. correct representation using averaging kernel and prior profiles used in the retrieval).
- **Observation space uncertainties:** assessed based on preliminary studies, justifiable
- **Prior fluxes and uncertainties:** promote use of open-access prior data and justifiable choices of prior uncertainty.
- **Boundary conditions:** promote use of open-access data and assessment of mixing ratio fields against independent observations.
- **Posterior uncertainty:** guidelines on a more complete assessment of posterior uncertainty through sensitivity tests.

Quality assurance

- **Report methodology:** develop protocol on how to report the methodology used
- **Report metrics:** determine key metrics to assess quality of posterior fluxes that should be reported, including more complete reporting of posterior uncertainty
- **Open-access:** promote open-access to code, prior information, and observations used to enable independent evaluation of the results.

Figure 4. Key elements for quality assurance



Best practice
Follow guidelines for atmospheric inverse modelling

Reporting
Clear reporting format and inclusion of metrics for quality of posterior fluxes

Open access
Use of open-access data and code to ensure reproducibility of results

Quality assurance
High-quality, traceable, and reproducible results

Summary and outlook

As interest in atmospheric inverse modelling for verifying national GHG emissions grows, a best practice will be essential to provide confidence in the estimates. The new Horizon Europe project, EYE-CLIMA (to start Jan-2023), will have a key component on the assessment of uncertainty in inverse modelling and how these should be reported. It will deliver best practice guidelines for inverse modelling and guidelines on how to compare these estimates to what is reported in national GHG inventories.