Figure xx (solid lines) shows the prior GEOS-Chem – TROPOMI difference with respect to albedo, season, and latitude for the filtered data. We find no bias with respect to albedo or season and an aseasonal latitudinal bias. This bias has been noted and corrected previously by Turner et al. (xxxx), Maasakkers et al. (xxxx), and Zhang et al. (xxxx). We define a latitudinal correction term (ppb) for the GEOS-Chem – TROPOMI difference using the first-order polynomial

where is the degrees latitude. We find good agreement between the resulting prior GEOS-Chem output and the observations (R = 0.77).

We also conduct a suite of sensitivity tests to provide additional constraints on the error of the optimized emissions, which are summarized in section 2.6.

We introduce a regularization factor (section 2.1) to account for the lack of covariance structure in . *[Isn’t there a source that says that scaling up the diagonal produces equivalent results to including off-diagonal elements?]* ….

Houweling et al. (2017):

“Errors that behave quasi-random and affect neighboring retrievals in a coherent way can in theory be accounted for by specifying the off-diagonal terms in the data error covariance matrix. In practice, there are many ways to do this, but quantitative information to justify a specific choice is lacking. In general, correlated uncertainty reduces the number of independent measurements, which justifies averaging retrievals within a certain distance of each other. Usually the uncertainty of the mean is calculated using a lower bound representing the contribution of purely systematic error. An alternative approach, referred to as ”error inflation”, is to increase the error of individually assimilated retrievals such that the uncertainty of a mean of surrounding retrievals does not drop below this minimum level (Chevallier, 2007). The advantage of this approach is that it avoids subjective decisions about which samples to combine into an average. Error inflation, or similar methods that compensate the neglect of off diagonals in the data error covariance matrix by increasing the (diagonal) uncertainty, lead to a χ 2 below 1. Although this may seem suboptimal from a statistical point of view, Chevallier (2007) demonstrated that this de-weighing of data nevertheless leads to uncertainty reductions that are closer to those obtained when off diagonals in R had been accounted for. Therefore, this approach avoids over constraining the problem by neglecting the contribution of data error covariance.”

“Observational error covariances are prescribed as the relative residual standard deviation of the column mismatch between the true-state synthetic observations and the prior simulations over a 2◦ × 2 ◦ moving window (Heald et al., 2004). We impose on the derived values a lower limit of 60 ppb2 , corresponding to the 0.25 quantile of the overall error distribution. The resulting observing system errors average 9 ppb (range: 8–29 ppb) and mainly reflect instrument noise. The 9 ppb estimate is in line with and slightly smaller than observational error estimates for previous methane inversions using data from TROPOMI (e.g., 11 ppb; Zhang et al., 2020) and GOSAT (e.g., 13 ppb; Maasakkers et al., 2019); it is therefore an appropriate representation for our OSSE analyses. Note that any systematic measurement errors (Lorente et al., 2021) are inherently not accounted for in our framework and would need separate correction.” (Yu et al. 2021)

“This reflects a tendency for SF inversions to overcorrect large sources while undercorrecting small sources (along with the fact that the satellite data themselves are less sensitive to small sources).” (Yu et al. 2021)

🡪 ask Daniel about this

“The U-SF inversion has DOFS = 382, with derived posterior error reductions that reflect the TROPOMI spatial sampling density for this month (Fig. 7). However, this computed error reduction ρest (derived via gradient-based randomization) has no meaningful spatial correlation with the actual emission improvement ρtrue (R = 0.07). This reflects the fact that the posterior error reductions and DOFS contain no information on where the prior emissions are actually in error and can therefore be improved. For a scenario where the prior emissions had random and normally distributed disparities relative to the truth, areas with the largest computed posterior error reduction would also tend to have the greatest emission improvement – since those locations would have the strongest observational constraints. DOFS and error reduction analyses are thus useful for general observing system characterization but do not describe the spatial accuracy of posterior emissions or the actual emission improvements for realistic scenarios where the real prior errors are nonrandom.”

🡪 ask Daniel about this

Often see better performance for small sources than large sources, since prior errors are probably more appropriate for small sources than for large sources (can cite Yu et al. to explain why Permian estimates may be too low)

We optimize 3653 grid cells and obtain 558 DOFS in CONUS, with smaller total corrected areas in Mexico (462 grid cells and 88 DOFS) and Canada (380 grid cells and 56 DOFS).

All modelled pathways that limit global warming to 1.5°C require deep reductions in methane emissions (IPCC). Yet, global methane concentrations have tripled from pre-industrial concentrations and are increasing at an increasing rate (Dlugokencky). Methane is emitted by a range of sectors, including the fossil fuel industry, livestock, waste management, and wetlands, the main biogenic source. Canada, the United States, and Mexico report their total estimated anthropogenic methane emissions to the United Nations Framework Convention on Climate Change (UNFCCC) using methods defined by the International Panel on Climate Change (IPCC). These “bottom-up” approaches combine activity data (e.g., number of natural gas pipelines) with emission factors (e.g., the leakage rate per pipeline) to estimate total emissions. However, significant uncertainties exist in both the spatial and temporal variability of emission factors, leading to large uncertainties in total and sectoral methane emission estimates. Satellite observations of atmospheric methane concentrations can improve bottom-up estimates with increasing sectoral accuracy through high-resolution inverse analyses (Streets et al. 2013, Jacob et al. 2016). We evaluate gridded versions of the national inventories of Canada, the United States, and Mexico for 2019 using observations of column methane concentrations from the TROPOspheric Monitoring Instrument (TROPOMI) aboard the Sentinel-5 Precursor. We estimate methane emissions at 0.25° ⨉ 0.3125° resolution, allowing for improved hotspot identification and source attribution.

The posterior solution depends on the choice of inversion parameters, including the prior emissions estimate, prior errors, the selection of observations, and the observing system errors. We solve the inversion for a range of

. The reduced-rank Jacobian matrix (section 2.6) optimizes emissions only in those grid cells that are informed by the observing system and defaults to the prior elsewhere.

together with the regularization factor (section 2.5) so that the prior term of the cost function evaluated at the posterior solution averages to 1 across all optimized grid cells (