



Constraints on methane emissions from geostationary observations

N. Bousseret et al.

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Constraints on methane emissions in North America from future geostationary remote sensing measurements

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Abstract

The success of future geostationary (GEO) satellite observation missions depends on our ability to design instruments that address their key scientific objectives. In this study, an Observation System Simulation Experiment (OSSE) is performed to quantify the constraints on methane (CH_4) emissions in North America obtained from Short Wave Infrared (SWIR), Thermal Infrared (TIR) and multi-spectral measurements in geostationary orbit compared to existing SWIR low earth (LEO) measurements. A stochastic algorithm is used to compute the information content of a variational inversion at high spatial resolution ($0.5^\circ \times 0.7^\circ$) using the GEOS-Chem chemical transport model and its adjoint. Both the SWIR LEO and TIR GEO configurations generally provide poor constraints on CH_4 emissions (error reduction $< 30\%$), with the exception of a few hotspots (e.g., Los Angeles, Toronto urban areas and Appalachian Mountains) where the error reduction is greater than 50% . On weekly time scales and for a GEO orbit, the degree of freedom for signal (DOFs) of the inversion from multi-spectral observations (500) is a factor of two higher than that obtained from a SWIR instrument (255) due to the increase in measurement sensitivity to boundary layer concentrations in the multi-spectral case. On a monthly time scale and for a GEO orbit, a SWIR instrument would reduce error in emission estimates by more than 70% for hotspots of CH_4 sources (emissions $> 4 \times 10^5 \text{ kg day}^{-1} \text{ grid}^{-1}$) at model grid scale, while a TIR instrument would provide a relative error reduction of $25\text{--}60\%$ over those areas. While performing similarly for monthly inversions, a multi-spectral instrument would allow for more than 70% error reduction for these emissions for 7 or 3 day inversions. Sensitivity of the inversions to error in boundary conditions are found to be negligible. Moreover, estimates of the model resolution matrix over significant emitting regions (CH_4 emissions $> 2 \times 10^5 \text{ kg day}^{-1} \text{ grid}^{-1}$) show that for all instrument configurations in GEO orbit the inversion is able to independently constrain CH_4 sources at spatial scales smaller than 200 km . These results highlight the importance of using observations sensitive

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to boundary layer concentrations (i.e., SWIR) to achieve significant improvements in constraining CH₄ sources compared to current LEO capabilities.

1 Introduction

Methane (CH₄) plays a key role in both atmospheric chemistry composition and climate. With a radiative forcing relative to preindustrial times that is one third that of carbon dioxide, CH₄ is the second most important greenhouse gas (Myhre, 2013). Further, as a precursor to tropospheric ozone, CH₄ also impacts surface-level air quality (Fiore et al., 2002; West et al., 2006; West and Fiore, 2005), crops (e.g., Shindell et al., 2012) and contributes to ozone radiative forcing (e.g., Fiore et al., 2008). Considerable uncertainty remains in our understanding of CH₄ sources (e.g., Dlugokencky et al., 2011; Kirschke et al., 2013), which include emissions from coal, wetlands, livestock, landfills, biomass burning, geologic seepage, and leaks from the production and distribution of natural gas.

Although there is a growing interest in using CH₄ emission regulations as an efficient lever to simultaneously address current air quality and global warming challenges (e.g., West et al., 2012), the lack of confidence in the available CH₄ emission estimates remains a problematic limitation to design of efficient environmental policies. Indeed, recent studies showed discrepancies of up to a factor of two between bottom-up inventories and top-down inversions using atmospheric CH₄ concentration observations (Katzenstein et al., 2003; Kort et al., 2008; Xiao et al., 2008; Karion et al., 2013; Miller et al., 2013; Wecht et al., 2012; Caulton et al., 2014; Turner et al., 2015; Wecht et al., 2014a). Extrapolation of local emission characteristics to larger areas and/or the use of proxy data (e.g., energy consumption, emission ratios applied to co-emitted species) are the main sources of error in bottom-up methods (Zhen et al., 2015). On the other hand, top-down approaches using space-based measurements of CH₄ from Low Earth Orbit (LEO) platforms allow a global spatial coverage within one to six days but at the same local time. However, as CH₄ emissions can exhibit significant diurnal cycles, e.g.,

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over wetland or boreal peatland (Morin et al., 2014; Gazovic et al., 2010), such temporal under sampling may affect our ability to accurately quantify those fluxes. More generally, insufficient observational coverage and the diffusive nature of transport considerably reduce our ability to spatially resolve grid-scale emissions from space.

5 Geostationary (GEO) remote-sensing measurements would alleviate the above mentioned shortcomings by providing an almost continuous monitoring and complete spatial coverage of CH₄ concentrations within the field of view. The GEOstationary Coastal and Air Pollution Events (GEO-CAPE) mission (Fishman et al., 2012) was recommended by the National Research Council's Earth Science Decadal Survey in order
10 to improve our understanding of both coastal ecosystems and air-quality from regional to continental scale. Its aim is to enable multiple daily observations of key atmospheric and oceanic constituents over North and South America from a GEO platform. For air-quality applications, such high-spatial and high-temporal-resolution measurements would enable source estimates of air quality pollutants and climate forcers and development of effective emission-control strategies at an unprecedented level of confidence.
15 In order to provide more flexibility and to minimize the cost and risk of the mission, the concept of a phased implementation that would launch remote-sensing instruments separately on commercial host spacecrafts has been adopted. The first phase will consist of the launching of the Tropospheric Emissions: Monitoring of Pollution (TEMPO)
20 instrument circa 2019 (Chance et al., 2013), which will provide GEO hourly measurements of ozone and precursors as well as aerosols over greater North America (from Mexico City to the Canadian tar sands, and from the Atlantic to the Pacific ocean). For the second phase, which aims at completing GEO-CAPE's mission requirements by including measurements of important drivers of climate and air quality such as CH₄, CO, and ammonia (Zhu et al., 2015), a rigorous instrument design study is critical to
25 achieve the mission's scientific objectives within its budget constraints.

In this study we perform an Observation System Simulation Experiment (OSSE) in order to characterize the constraints on grid-scale CH₄ emissions over North America provided by different potential GEO-CAPE instrument configurations. The simulation

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consists of a 4D-Var inversion of CH₄ emissions using the GEOS-Chem chemical-transport model (CTM) over a 0.5° × 0.7° horizontal grid resolution covering North America. In practice, quantifying the information content of such a high-dimensional problem requires either Monte-Carlo simulations or, for linear models, a numerical approximation of the inverse Hessian matrix of the 4D-Var cost function (Tarantola, 2005). The computational cost of Monte-Carlo estimates can be prohibitive, since many perturbed inversions (typically about 50) are needed, each of them usually requiring numerous forward and adjoint model integrations. Therefore, computation of the information content in previous trace-gas Bayesian inversion studies has often relied on explicit calculations of the inverse Hessian matrix, by either considering a regional domain (e.g., Wecht et al., 2014a) or performing a prior dimension reduction of the control vector (e.g., Wecht et al., 2014b; Turner and Jacob, 2015). However, thus far dimension reduction methods for high-dimensional emission inversions have relied on suboptimal criteria.

In this study we use a gradient-based randomization algorithm to approximate the inverse Hessian of the cost function (Bousseret et al., 2015), which allows us to calculate the posterior errors as well as the model resolution matrix (or averaging kernel) of our CH₄ emission inversion at full grid-scale resolution. Such information is used to evaluate the impact of different instrumental designs (spatio-temporal sampling, vertical sensitivity of the measurements) on CH₄ emission constraints. In particular, the potential of CH₄ retrievals from existing Short Wave Infrared (SWIR) and Thermal Infrared (TIR) measurements as well as from a hypothetical multi-spectral instrument on geostationary orbit are examined. Section 2 describes the Observing System Simulation Experiment (OSSE) framework considered in this study, which comprises the 4D-Var method, the forward model, as well as the observations and prior information used. Section 3 presents the results of our experiments, where the information content of the inversion is analyzed in detail. A conclusion to this work is presented in the last section of the paper.

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This equivalence can be used to compute information content diagnostics prior to performing the inversion. In this study, following Bousseret et al. (2015), the diagonal elements of \mathbf{P}^a (error variances) are computed using a randomization estimate of $\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}$. Here an ensemble of 500 random gradients of the cost function are used, based on the convergence of the uniform norm ($\|\cdot\|_\infty$) of the inverse Hessian approximation. Bousseret et al. (2015) showed that good approximation of both the error variances and the error correlations can be obtained using this approach. For the present study we further validated our method by comparing direct finite-difference estimates of selected diagonal elements of \mathbf{P}^a to their stochastic approximations and found a relative error smaller than 10 %.

The model resolution matrix (or averaging kernel \mathbf{A}) is defined as the sensitivity of the analysis \mathbf{x}_a (optimized CH_4 emissions) to the truth \mathbf{x}_t (true emissions):

$$\mathbf{A} \equiv \frac{\partial \mathbf{x}_a}{\partial \mathbf{x}_t}. \quad (4)$$

The model resolution matrix in Eq. (4) can be rewritten in matrix form:

$$\mathbf{A} = \mathbf{I} - \mathbf{P}^a \mathbf{B}^{-1}. \quad (5)$$

Since \mathbf{B} is diagonal in our experiments, Eq. (5) allows us to calculate any element of \mathbf{A} using:

$$\mathbf{A}_{i,j} = \delta_{ij} - \frac{\mathbf{P}_{i,j}^a}{\mathbf{B}_{j,j}}. \quad (6)$$

Finally, the degree of freedom for signal (DOFs) of the inversion is defined as the trace of \mathbf{A} , that is: $\text{DOFs} = \sum_i \mathbf{A}_{i,i}$.

2.2 Forward model and prior emissions

The forward model in Eq. (1) includes the GEOS-Chem chemistry-transport model, which relates the CH_4 emissions to the 3-D concentration field of atmospheric CH_4 ,

trations and aircraft-based observations from the HIAPER Pole-to-Pole Observations (HIPPO) experiment (Turner et al., 2015). These results show that a 2 % positive perturbation of the boundary conditions results in absolute posterior emission scaling factor responses smaller than 0.05 for all observational configurations. Moreover, the noisy characteristic of the scaling factor perturbations is evident for all inversions. Therefore, errors in boundary conditions of a few percent or less are found to have a negligible impact on our CH₄ source inversions.

3.3 Spatial resolution of the inversion

An objective measure of the spatial resolution of the inversion, i.e., the ability of the observational system to constrain grid-scale emissions independently from each other, is provided by the rows of the model resolution matrix (see Eq. 5). Figure 7 shows the model resolution matrix rows corresponding to five different locations, chosen to span a range of characteristics, in terms of emissions magnitude and error reduction. Table 1 summarizes the coordinates and CH₄ emissions corresponding to each location. The gain in spatial resolution as the sensitivity of the retrieval to boundary layer CH₄ concentrations increases is evident, especially for eastern Canadian wetlands and the Los Angeles area. For all instrument configurations, observations allow for constraints on CH₄ emissions at spatial resolutions between 80 km × 80 km and 160 km × 160 km. Note that over regions such as the wetlands in eastern Canada, the Appalachian Mountains and the Los Angeles area, using a multi-spectral instrument from geostationary orbit would allow complete constraints of CH₄ sources at grid-scale resolution (0.5° × 0.7°).

4 Conclusions

In this paper we evaluated top-down constraints on methane emissions in North America provided by potential geostationary observation missions (GEO-CAPE) and existing low-earth orbit remote sensing instruments (GOSAT). For the first time, a rigorous es-

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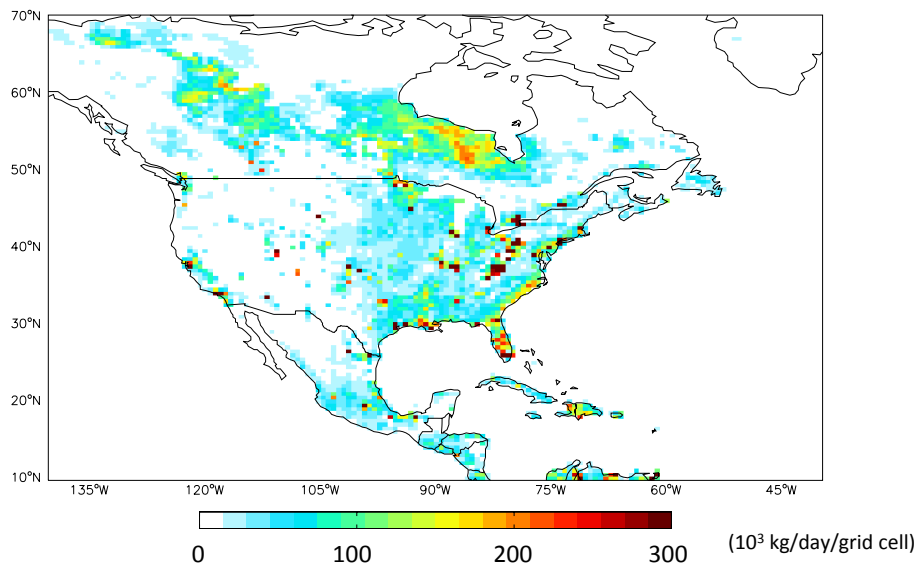


Figure 1. Total average daily prior methane emissions for the nested North America domain ($0.5^\circ \times 0.7^\circ$).

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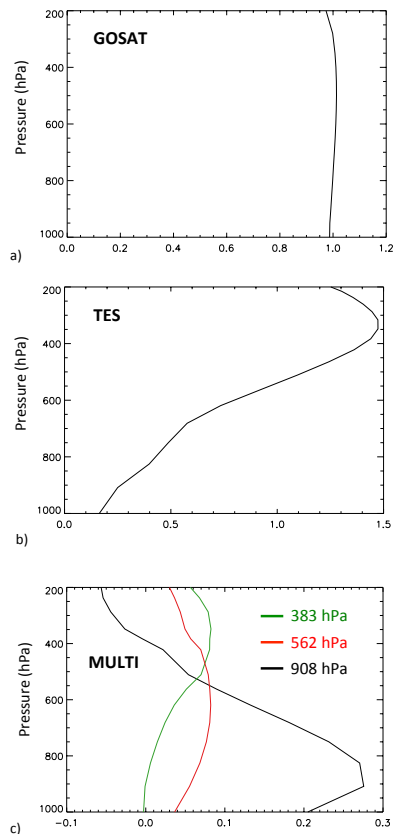
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Figure 2. Averaging kernels for the different instrument configurations: **(a)** GOSAT column averaging kernel; **(b)** TES column averaging kernel; **(c)** Multi-spectral averaging kernels at three pressure levels: 908, 562 and 383 hPa.

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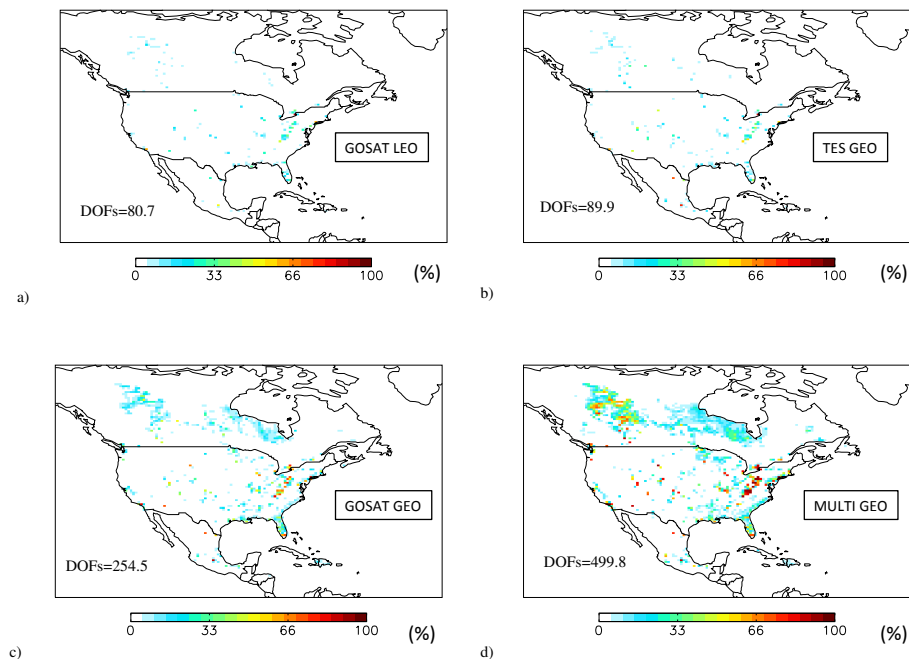


Figure 3. Reduction (%) in methane emission standard errors for a 7 day inversion (1–8 July 2008) using: **(a)** GOSAT low-earth orbit observations (GOSAT_LEO); **(b)** GEO-CAPE observations with a TES-like instrument (TES_GEO); **(c)** GEO-CAPE observations with a GOSAT-like instrument (GOSAT_GEO); **(d)** GEO-CAPE observations with a multi-spectral instrument (MULTI_GEO). The degree of freedom for signal (DOFs) of each inversion is also indicated.

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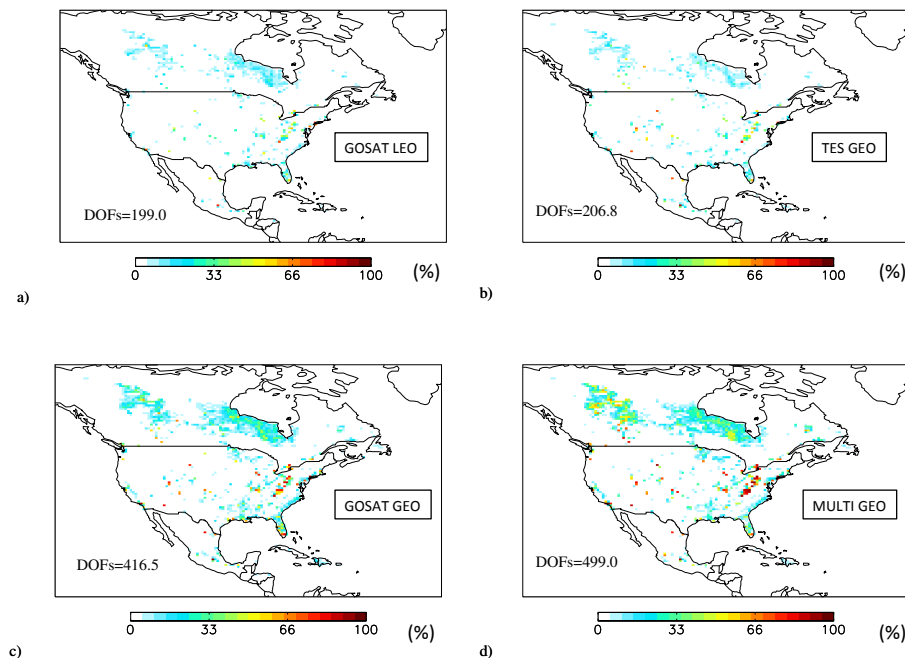


Figure 4. Reduction (%) in methane emission standard errors for a 30 day inversion (1–30 July 2008) using: **(a)** GOSAT low-earth orbit observations (GOSAT_LEO); **(b)** GEO-CAPE observations with a TES-like instrument (TES_GEO); **(c)** GEO-CAPE observations with a GOSAT-like instrument (GOSAT_GEO); **(d)** GEO-CAPE observations with a multi-spectral instrument (MULTI_GEO). The degree of freedom for signal (DOFs) of the inversion is also indicated.

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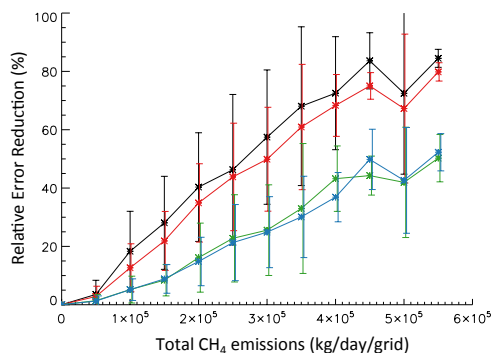
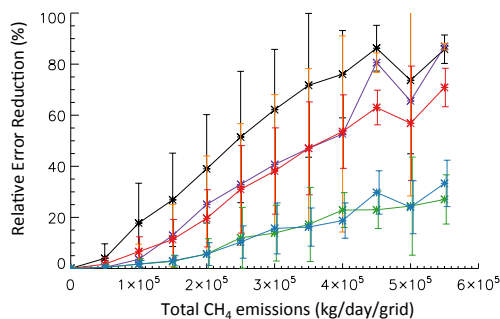


Figure 5. Reduction (%) in methane emission standard errors as a function of emission magnitude for a 7 day (1–8 July 2008) (top) and a 30 day (1–30 July 2008) (bottom) inversion. Blue: GOSAT low-earth orbit observations (GOSAT_LEO); green: GEO-CAPE observations with a TES-like instrument (TES_GEO); red: GEO-CAPE observations with a GOSAT-like instrument (GOSAT_GEO); black: GEO-CAPE observations with a multi-spectral instrument (MULTI_GEO). Results for a 3 day MULTI_GEO inversion are also shown in purple (top). The vertical bars indicate the standard deviation of the relative error reduction within each bin.

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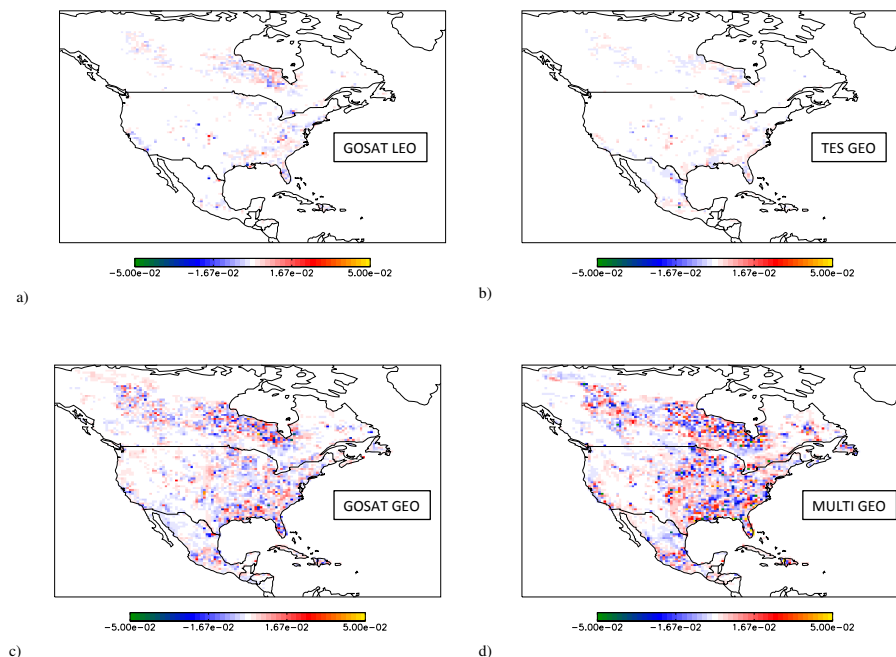


Figure 6. Sensitivity of optimized emission scaling factors (unitless) to a 2% perturbation of boundary condition methane concentrations for a 30 day inversion (1–30 July 2008), using: **(a)** GOSAT low-earth orbit observations (GOSAT_LEO); **(b)** GEO-CAPE observations with a TES-like instrument (TES_GEO); **(c)** GEO-CAPE observations with a GOSAT-like instrument (GOSAT_GEO); **(d)** GEO-CAPE observations with a multi-spectral instrument (MULTI_GEO).

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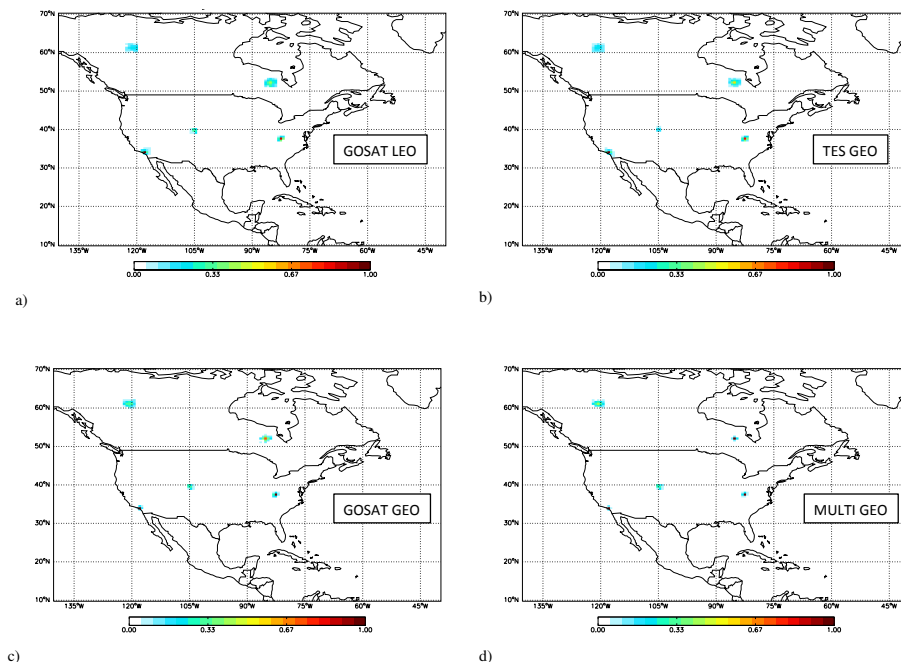


Figure 7. Rows of the model resolution matrix (unitless) for five locations for a 30 day inversion (1–30 July 2008), using: **(a)** GOSAT low-earth orbit observations (GOSAT_LEO); **(b)** GEO-CAPE observations with a TES-like instrument (TES_GEO); **(c)** GEO-CAPE observations with a GOSAT-like instrument (GOSAT_GEO); **(d)** GEO-CAPE observations with a multi-spectral instrument (MULTI_GEO). Coordinates of the five locations considered are reported in Table 1 and correspond to the center of each structure on the maps.

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