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Quantification of methane emissions from hotspots and during COVID-19 using a global atmospheric inversion

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The full list of simulations performed are provided in ST1 with the dates and purpose of the experiment, these can be divided between those used for prior error tuning and those used for source attribution for different times.

Experiment Name	Start Date	End Date	Purpose
PR_10	1st May 2019	1st June 2019	Evaluate 10% prior error
PR_20	1st May 2019	1st June 2019	Evaluate 20% prior error
PR_40	1st May 2019	1st June 2019	Evaluate 40% prior error
PR_80	1st May 2019	1st June 2019	Evaluate 80% prior error
PR_MAP	1st May 2019	1st June 2019	Evaluate mapped error
PR_MAP_0.5	1st May 2019	1st June 2019	Evaluate halved mapped error
Control_AN	1st May 2019	1st June 2019	Control Analysis for Comparison
INV_2018	1st May 2018	1st July 2018	Emissions for 2018 (including case studies)
INV_2019	1st January 2019	1st July 2019	Emissions for 2019 (including case studies)
INV_2020	1st January 2020	1st July 2020	Emissions for 2020 (including case studies)
EAG_2019	1st October 2019	1st December 2019	Eagle Ford blowout case study
LATE_2020	1st August 2020	31st December 2020	Various case studies.

Table S1: Details of all IFS inversion experiments performed.

The global coverage of TROPOMI XCH_4 is represented for a single day in S1, data have been gridded to the IFS increment resolution (~40km^2) and averaged where multiple observations are available. The coverage is representative of the number of quality checked observations assimilated within one 24-window (~150,000). GOSAT and IASI observations are also assimilated further improving the global coverage.

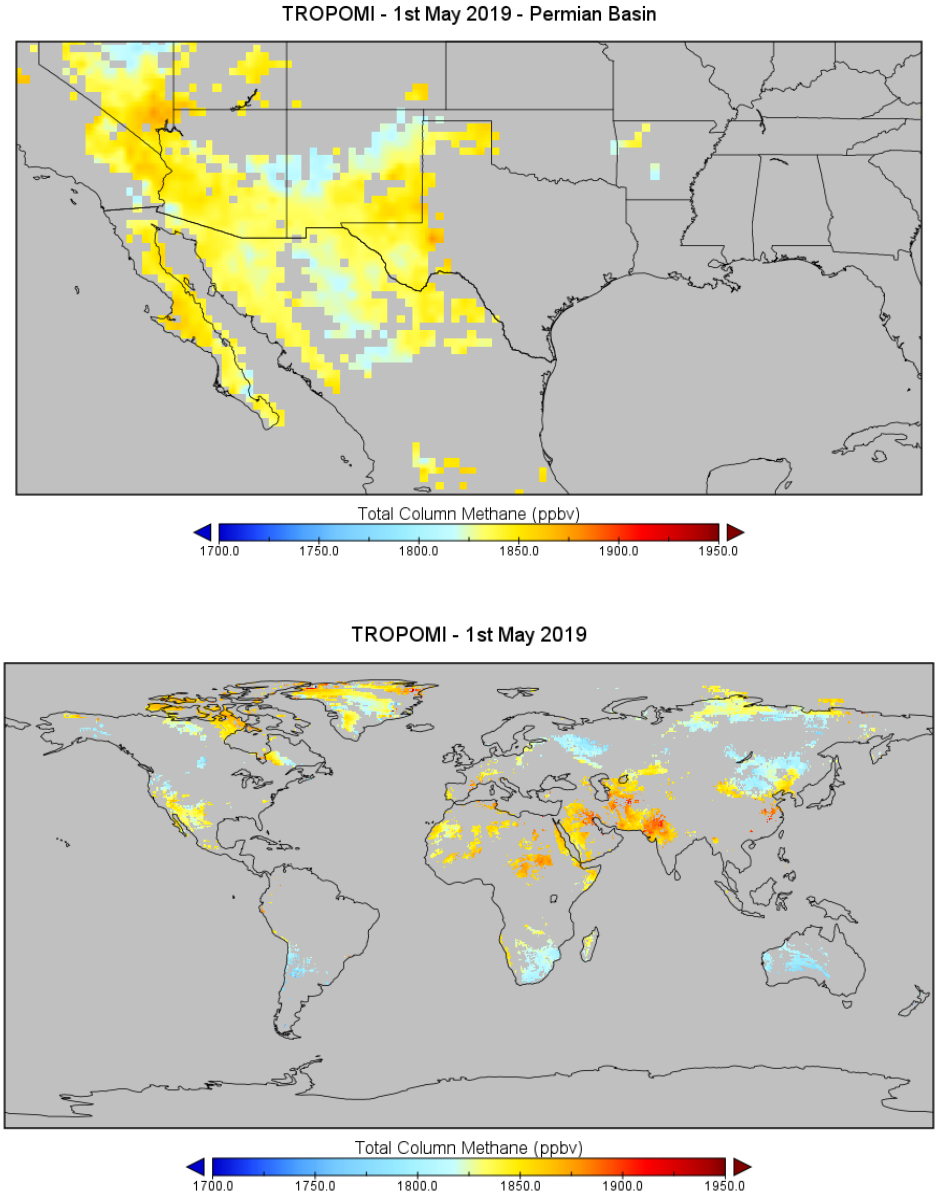

Figure S1: Example TROPOMI XCH_4 coverage for a 24-hour period on 1st May 2019. Maximum stringency quality flags are applied to remove poor data. Note that observations are averaged into 40 km^2 gridcells.

Prior error evaluation was performed using multiple estimates as given by table S1 (PR_*). Comparisons were made for a 1-month period (May 2019) with TCCON retrievals (Wunch *et al.*, 2011) (S2). Only a subset of the 16 sites are shown for illustration purposes. Averaged across all sites the lowest standard error and absolute mean bias, and high correlation was found when using the mapped prior error (PR_MAP).

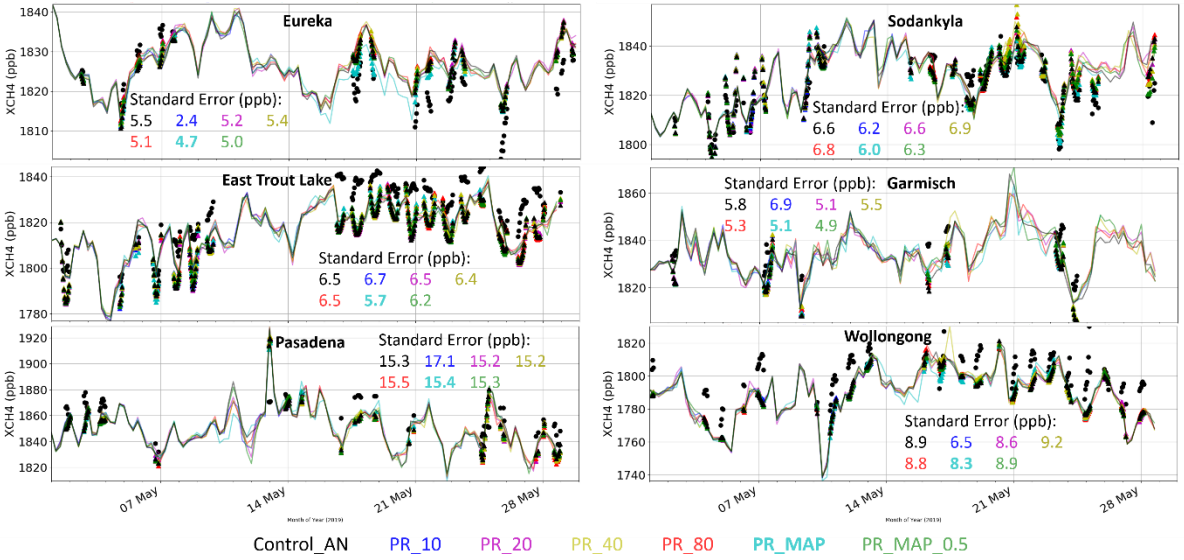

Figure S2: Comparisons of XCH_4 from inversions using 6 different prior uncertainties and 1 where only the initial 3d-state is optimised (Control_AN) with a subset of 6/16 TCCON sites for May 2019 with standard error values given.

A climatological background error is used for the initial CH_4 3D state in the 4D-Var inversion, this is fixed in time and shown as a global average profile in S3.

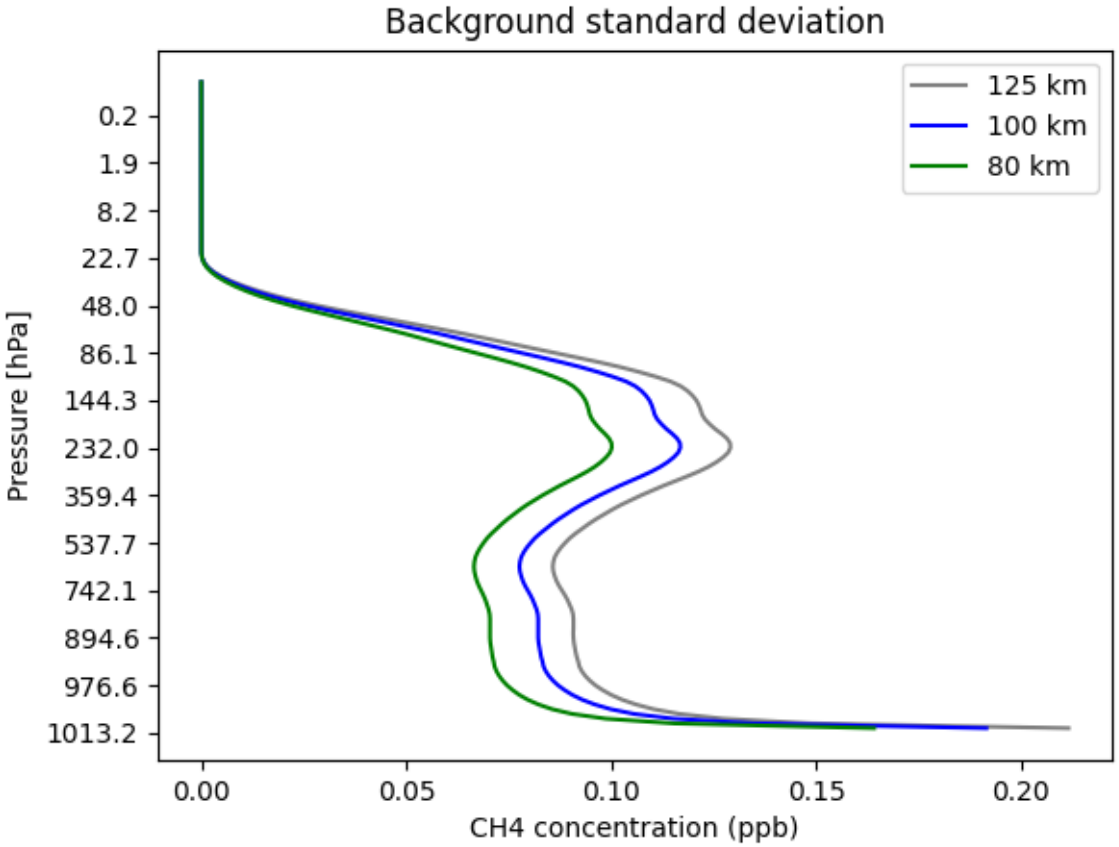

Figure S3: Climatological background standard deviation of CH_4 at 3 different model resolutions. The profiles represent global averages.