Response to reviewers (2nd round of revisions)

Quantifying CO emissions from boreal wildfires by assimilating TROPOMI and TCCON observations

Our responses to the referee comments and updates in the revised manuscript are listed below. Referee comments are in black and author responses are in blue. The line numbers in our responses refer to the 2nd revised manuscript.

Referee 3 (RC3):

The revised manuscript was significantly improved by the authors. All comments were sufficiently replied to and the manuscript was modified accordingly. I'm happy to accept the manuscript for publications with just a few very minor suggestions with all except one being purely technical:

minor:

- 1.350-355: Thank you for adding additional information on the ensemble generation. For me it is not entirely clear if the perturbations of each member are sampled uniformly (i.e. one emission perturbation factor for each member applied globally throughout the whole time period) or vary in space and time (if so, are they spatio-temporally correlated?)? Please describe.

Thank you for your question and the opportunity to clarify. The perturbation of the emission scaling factors for ensemble generation is performed within the CHEEREIO framework. In our setup, the scaling factors are initialized randomly at the grid scale for each ensemble member, meaning that perturbations vary spatially rather than being applied uniformly or globally. These perturbations are sampled from a multivariate lognormal distribution, with spatial correlations imposed using an exponential decay function with a correlation distance of 500 km. We assume no explicit temporal correlations. Therefore, the spatially varying and correlated scaling factors are initialized at the beginning of the assimilation window for each ensemble member and are subsequently updated by observation increments at every assimilation cycle (3-day).

Further details on ensemble generation can be found in Section 3.2 of Pendergrass et al. (2023), and a description of the scaling factor perturbations is provided in the CHEEREIO documentation:

 $\underline{https://cheereio.readthedocs.io/en/latest/The-ensemble-configuration-file.html?highlight=perturb\#scaling-factor-settings.}$

Text revised and added in Section 3

(lines 326-329):

"To obtain a posteriori estimate of CO emissions, we begin by initializing the ensemble scaling factors using a multiplicative random perturbation to the prior estimates from all emission sources at the grid scale (i.e., spatially varying perturbations), sampled from a multivariate lognormal distribution (see the detailed description of ensemble generation in Pendergrass et al. (2023), Section 3.2)."

(lines 348-354):

"Then, an ensemble spin-up without assimilating observations is performed, where emissions are randomly perturbed at each grid point based on a lognormal distribution to create an ensemble spread. We assume a lognormal standard deviation of $\sigma = 0.2$, centered around 1, that provides ensemble member scaling factors between 0.55 and 1.82 with 99% confidence. This perturbation level is sufficient to generate meaningful ensemble spread while avoiding unrealistically high or low values for constructing the prior error covariance. The scaling factors are assumed to be spatially correlated using an exponential decay function with a correlation distance of 500 km, while no explicit temporal correlations are imposed."

technical:

- 1.145: Does "same TCCON data" refer to the assimilated data? I would suggest replacing "same" with "assimilated" Yes, "same TCCON data" refers to the assimilated data. We have revised the text as suggested in Section 2 (line 146).

- 1.154: "a local overpass solar times" is there a word missing? Or inconsistency between singular ("a") and plural ("times")

Corrected. We have revised the text in Section 2.1 (line 154): "a local overpass solar time of 13:30 UTC"

- 1.330ff and 355ff: Due to the changes in 1.330ff, this sentence is now doubled with almost identical content. Please remove one of them.

Thanks for pointing this out. We have removed the second occurrence of similar content regarding the use of the lognormal distribution in Section 3 (line 356): "The choice of a lognormal distribution not only maintains the positivity of the solution (i.e., prevent an unrealistic negative scaling factors), but also better represents the uncertainty of CO emission estimates from inventories (Maasakkers et al., 2019; Plant et al., 2022)."

Additional minor updates:

- 1. Updated Fig. 4c and 4i to remove a duplicate label in the subfigures.
- 2. Line 108: replaced ", and therefore" with "; therefore,".
- 3. Line 116: replaced "The TCCON" with "TCCON".
- 4. Line 149: replaced "inversion's setup" with "inversion setup".
- 5. Line 167: replaced "within" with "in".
- 6. Lines 179-180: replaced "reports" with "report shows that".
- 7. Line 180: added "data" after "XCO".
- 8. Figure 1 caption: replaced "The number" with "Number"; "quality controlled" with "quality-controlled"; "The variability" with "Variability"; "Temporal series" with "Time series"; and removed repeated "East Trout Lake" and repeated "column averaging kernels".
- 9. Line 222: removed "(see Table 2)".
- 10. Line 288: replaced "vegetation-type" with "vegetation type".
- 11. Line 289: replaced "Global" with "the Global".
- 12. Line 300: replaced "averaged" with "average".
- 13. Line 306: replaced "has" with "have".
- 14. Line 303: replaced "satellite driven" with "satellite-driven".
- 15. Line 308: replaced "global gridded" with "globally gridded".
- 16. Line 312: added "the" before "background".
- 17. Line 315: replaced "detail" with "detailed".
- 18. Line 324: replaced "location and time" with "locations and times".
- 19. Line 335: replaced "by" with "of".
- 20. Line 336: replaced "LETKF" with "the LETKF".
- 21. Line 339: removed "the" before "BB".
- 22. Line 351: replaced "between 0.55 to 1.82" with "between 0.55 and 1.82".
- 23. Line 356: replaced "perturbation of emissions" with "perturbations in emissions".
- 24. Line 367: replaced " $\Delta = 0.08$ " with " $(\Delta = 0.08)$ "; and "quick" with "rapid".
- 25. Line 368: replaced "which may result in an inversion not being updated" with "which may otherwise prevent the inversion from being updated".
- 26. Line 370: replaced "impacted" with "affected".
- 27. Line 403: replaced "into" with "in".
- 28. Line 449: added "the" before "joint inversion".
- 29. Line 450: replaced "assimilation" with "inversion".
- 30. Line 452: added "could" before "benefit".

- 31. Line 454: replaced "emission" with "emissions"; and "between all the inventories" with "across all inventories".
- 32. Line 458: removed "of the".
- 33. Line 459: replaced "increases to" with "reaches".
- 34. Line 460: removed 'of uncertainty".
- 35. Line 502: replaced "Fig. 3d,i,n" with "Fig. 3b,g,l,d,i,n".
- 36. Figure 6 caption: replaced "inversion (red)" with "(red) inversions"
- 37. Line 573: replaced "the vector of dimension, m" with "a vector of dimension m"; and added "the" before "number".
- 38. Line 584: replaced "inversion" with "inversions".
- 39. Line 596: replaced "inversion" with "inversions".
- 40. Line 598: replaced "improves" with "improve".
- 41. Line 600: replaced "assimilation" with "assimilations".
- 42. Line 601: replaced "timeseries with "time series"; and "shows" with "show".
- 43. Line 605: replaced "show" with "shows".
- 44. Figure 7 caption: replaced "of all sites" with "for all sites"; "a timeseries and scatter plot" with "time series and scatter plots"; "however" with "but"; and "estimate" with "estimates".
- 45. Figure 8 caption: replaced "from bottom-up inventories" with "inventory"; added "the" before "prior" and "posterior".
- 46. Line 628: added "a" before "further".
- 47. Line 638: added "the" before "model"; and replaced "are" with "is".
- 48. Line 641: added "estimates" after "a posteriori"; and replaced "we see" with "observed".
- 49. Line 637 and 644: replaced "2°×2.5°" with "2° × 2.5°".
- 50. Line 644: replaced "for" with "at the".
- 51. Line 649: replaced "most of the cases" with "most cases".
- 52. Line 650: replaced "to the bias of the" with "to that of the".
- 53. Line 651: replaced "an equivalent ... estimate" with "equivalent ... estimates".
- 54. Line 658: added "the" before "a posteriori"; removed "time" before "period".
- 55. Figure 9 caption: added "the" before "a priori" and "a posteriori"; replaced "between" with "for"; replaced "of" with "between"; and added "for" before "comparison".
- 56. Line 672: replaced "assimilation" with "estimate"; and replaced "with" with "for".
- 57. Line 676: added "estimates" after "XCO"; removed "i.e.," in the parentheses.
- 58. Lines 676-677: shifted "than those with QFED and GBBEPx" to the end of the sentence.
- 59. Line 677: replaced "mode estimated" with "model-estimated"; replaced "has" with "shows".
- 60. Line 680: replaced "while" with "whereas".
- 61. Line 693: removed "of extreme wildfires".
- 62. Line 703: replaced "CFEEPS" with "CFFEPS".
- 63. Figure 10 caption: removed "the" before "prior"; added "profiles" after "a priori".
- 64. Figure 11 caption: replaced "preformed" with "performed"; added "TCCON" before "XCO"; added "data" after "TROPOMI-only" and replaced "a joint TROPOMI and TCCON" with "joint TROPOMI and TCCON data".
- 65. Lines 723-724: added "estimates" after "a priori"; removed "have".
- 66. Line 727: replaced "a closer estimate" with "closer estimates".
- 67. Line 731: replaced "with matching variability with the measurements" with "with variability matching the measurements".
- 68. Line 739: replaced "grided" with "gridded".
- 69. Line 748: replaced "Colombia" with "Columbia".
- 70. Figure 12 caption: added "the" before "CFFEPS"; replaced "TROPOMI and TCCON standard XCO TCCON" with "TROPOMI and standard TCCON"; and removed "XCO" before "TCCON".

- 71. Lines 758-760: removed "in" before the color names in parentheses.
- 72. Line 761: removed "the" before "inversion cases".
- 73. Figure 13 caption: replaced "Evaluating" with "Evaluation of"; replaced "of" with "from"; added "the" before "a priori".
- 74. Line 773: replaced "due" with "due to".
- 75. Lines 791-792: replaced "plume" and "altitude" with "plumes" and "altitudes".
- 76. Line 805: replaced "column averaged" with "column-averaged".
- 77. Line 818: removed "between" after "by".
- 78. Lines 826: replaced "deference" and "standard deviation" with "differences" and "standard deviations"; added "the" before "assimilation".
- 79. 847-848: replaced "inversions" with "inversion"; and "improve" with "improves".
- 80. Lines 860: replaced "an idealized condition" with "idealized conditions".
- 81. Figure A1 caption: replaced "true prior" with "prior true"; replaced the second occurrence of "(c)" with "(d)".
- 82. Line 876: replaced "and" with "under".
- 83. Line 878: added "the" before "assimilation parameter".
- 84. Lines 883: replaced "posterior" with "posteriors".
- 85. Line 894: added "only" before "TCCON".
- 86. Table B1 caption and footnotes: added "the" before "true emissions"; replaced "priror" with "prior"; and replaced "is" with "are".
- 87. Line 940: replaced "is" with "are".
- 88. Line 952: replaced "that" with ", which".
- 89. Line 956: replaced "QFEDv2.5r1" with "QFED v2.5r1".