

Atmos. Chem. Phys. Discuss., referee comment RC1
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Comment on acp-2021-474

Anonymous Referee #1

Referee comment on "A new inverse modeling approach for emission sources based on the DDM-3D and 3DVAR techniques: an application to air quality forecasts in the Beijing–Tianjin–Hebei region" by Xinghong Cheng et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2021-474-RC1>, 2021

General comments:

This study developed a new inverse modeling approach based on DDM-3D and 3DVAR, which was applied to assimilate surface SO₂ and NO₂ concentration measurements to optimize SO₂ and NO_x emissions in the Beijing-Tianjin-Hebei region. The a posteriori emission inventory is applied to air quality forecast, and results show the simulated surface SO₂, NO₂, and O₃ concentrations using the a posteriori emission inventory are in better agreement with observations than a priori. I will recommend its publication after the following comments are addressed.

Specific comments:

- Inversion modeling tools are summarized in the 3rd paragraph in the introduction, but how to classify them is open to discussion. Is it appropriate to consider adjoint modeling and sensitivity analysis as two inversion modeling tools? In the manuscript Stavrakou et al. (2009) and Zhai et al. (2018) are considered as adjoint modeling. The two references did use adjoint modeling, but actually (1) Stavrakou et al. (2009) used adjoint modeling to calculate sensitivity, which was future used to minimize a 4DVAR cost function; (2) Zhai et al. (2018) only used adjoint modeling to calculate sensitivity without constrain emissions. Thus, Stavrakou et al. (2009) should be considered as 4DVAR, and Zhai et al. (2018) should not be cited. I agree that Henze et al. (2009) and Jiang et al. (2011) should be classified as 4DVAR; the two papers used GEOS-Chem adjoint model to calculate the sensitivity of cost function with respect to emissions scale factors, and the sensitivity were used to minimize cost functions. Considering

sensitivity analysis as the name of inversion modelling is inappropriate as many approaches (such as 4DVAR) need to calculate sensitivity. Moreover, Mijling et al. (2012) was considered as sensitivity analysis in the manuscript, but actually it should be Kalman filter. I did not read all the references in the paragraph and could not help classify them; I suggest reading them carefully and classifying them properly.

- Line 86: The reason that GEOS-Chem is not used urban air quality forecast is its spatial resolution is too coarse, and I suggest add this explanation.
- Line 88-90: Why it is stated EnKF and 4DVAR are absent of sensitivity analysis of the source-receptor relationship? Adjoint model (for example, GEOS-Chem adjoint) is used to calculate the source-receptor relationship in 4DVAR.
- Line 115-118: Are there any references to show that multiple receptors will result in high computational costs for adjoint model? My experience is whether assimilating one species or multiple species, the computational time difference for calculating the cost functions with respect to emissions is very small.
- How the uncertainties in Table 1 are calculated? If they come from other paper, please add references.
- I suggest add some details of random perturbation method that is used to generate the 30 sets of inventories.
- Line 193: What "24-h strengths of ES for each month" mean?
- How a priori SO₂ and NO_x emissions are vertically distributed in the model?
- Please check Eq. (3) careful. Which p should or not be capitalized?

Technical corrections:

- Line 74: Henze et al., 2008 -> Henze et al., 2009. And the year is also wrong in the reference list.
- Please check Eq. (3) and corresponding descriptions carefully. Which p should or not be capitalized?