General comments

This paper presents a new method for estimating methane emission source location on oil and gas sites using in situ point sensors. The method combines a backward Lagrangian dispersion model (TERRAFEX) with a gradient-based method for isolating enhancements in the resulting concentration maps. The authors use this method to evaluate detection and localization performance of the in situ sensors via a simulation study, where artificial sensor data is generated using a Gaussian dispersion model. I believe that the results of this simulation study are the primary contribution of this work, as they may be able to provide performance bounds that could be expected in practice. The authors also apply the method to real data collected on an oil and gas facility.

However, I have a number of major concerns that must be addressed before I am able to fully interpret the proposed method, the simulation study, and the case study using real data. My primary concern is that the methods are not described in sufficient detail to be fully understood. For example, the description of the Gradient Indicator tool is lacking, and as such, it's not clear to me how this method picks an estimated source location based on output from the backward Lagrangian simulation tool. This makes it hard to evaluate the accuracy metrics presented in the results. Additionally, it's not clear if the main result tables (Tables 1-3) and figure (Figure 7) are for one of the source-sensor configurations used in the simulation study, or an average over all source-sensor configurations. This makes the results hard to interpret, as different configurations could have very different detection / localization capabilities. There also appear to be inconsistencies between Table 3 and Figure 7(b). Finally, I think that the writing could be refined; some ideas are expressed imprecisely making it hard to follow at times. See below for a complete list of comments.

Specific comments

- L58-59: The authors should note that gaps in CEMS detections are a result of wind blowing between sensors and that these periods can be identified (and subsequently addressed) by using an atmospheric dispersion model. For example, see: https://doi.org/10.1021/acs.estlett.4c00687
- L60-64: The authors should note that there is variability in localization and quantification performance across the commercial solutions studied in Bell et al. 2022 (and in the subsequent ADED evaluations, see https://doi.org/10.1021/acs.est.3c08511 and https://doi.org/10.1021/acs.est.3c08511 and https://doi.org/10.26434/chemrxiv-2024-f1znb-v2). Some commercial solutions struggle to localize emissions, as the authors note, but others perform this task relatively well when evaluated at METEC.
- L82-83: This is not entirely true, there are several open-source methods for CEMS inversions in the literature. See for example:
 https://doi.org/10.48550/arXiv.2506.03395,
 https://doi.org/10.1021/acsearthspacechem.2c00093,
 - https://doi.org/10.1525/elementa.2023.00110, https://doi.org/10.5194/amt-11-

- <u>1565-2018</u>. The authors are correct, however, that commercial CEMS solutions often do not make their algorithms completely open source.
- The concept of a footprint is discussed in the introduction and methods sections but is not fully defined. I recommend defining this term in the introduction given that it is a key idea in the manuscript.
- The concept of a "forward simulation" vs. a "backward simulation" should be defined in the introduction
- L145: "source weight function" is not defined.
- Second paragraph of 2.2. More detail about the GI method is necessary. I don't understand some key ideas from this paragraph (e.g., the x and y direction and the new vs. original matrices).
- Each box in Figure 1 needs more detail to be interpretable. I'm not sure what a lot of these boxes mean, even after reading the previous paragraphs in Section 2.2
- Section 2.2 would be aided by a Figure showing the concentration maps, and perhaps an example of a "hot spot"
- Figure 3 is not a "time series," as it is referred to on L271. A time series would plot the methane concentrations on the vertical axis with time on the horizontal axis. These plots show concentration as a function of wind direction.
- Fig 5: could there be other sources on this site besides the four you identified? If so, how would this impact the analysis? Some discussion of this point should be included.
- Fig 6: it's not clear which source-sensor configuration is being shown here. Are there many sensors along the x=0 line? Or just one at x=y=0?
- Fig 6: I'm not sure what the concentration field on the right is showing. I think more detail needs to be included in Section 2.1 when describing TERRAFEX, because it's not clear to me what the output from this model shows. Is it the estimated plume shape based solely on the sensor measurements? If so, why is the plume wider on the left and narrower on the right? Also, can the authors explain the other artifacts in this concentration field?
- Fig 6: It would be very useful to show where the GI method would identify the source given this concentration map.
- Table 1: Are these metrics averaged across all source-sensor configurations? If so, it would be very hard to interpret these numbers, as different arrangements may have very different detection characteristics.
- Figure 7: The 95% confidence interval almost spans the entire range of the POD parameter (0-1). Some discussion of this point should be included. How confident are you in these trends given the very large confidence intervals?
- Figure 7 Panel a: The stability classes are sorted so that the POD is increasing from low to high. This needs to be stated directly, otherwise this plot is misleading.
- Figure 7 Panel b: the 100 mark on the horizontal axis is not in the correct order. I think this is also plotted so that the POD is strictly increasing, which is misleading. The horizontal axis should be increasing distances.

- Figure 8: is one pixel selected as the source location estimate? Or is the entire red swath the source estimate? The red region covers the sources, but it also covers much of the rest of the site as well. How do you pick a source location from the concentration maps shown in this figure?
- The POD values in Tab 3 don't seem to line up with the values in Fig 7 panel C. This needs to be checked.

Technical corrections

- Localization accuracy (LA) acronym is defined twice in the abstract
- Methane is defined as "CH4" twice in the first paragraph of the introduction, but the authors continue to use "methane" throughout the paper.
- L53: Jia et al. 2023 has been published: https://doi.org/10.1038/s41598-025-99491-x
- L59: There is no Daniels et al. 2022 in the list of references. Do the authors mean to say Daniels et al. 2023 or Daniels et al. 2024?
- L71: The Gaussian puff and plume models studied in Jia et al. 2025 are not back-trajectory methods. They are forward models that simulate the transport of methane from the source to the sensor.
- L91-98: This discussion would be clearer if the authors first provide a clear definition of both "concentration footprint" and "flux footprint."
- L113: "localization" is defined here but used multiple times earlier in the introduction. It should be defined at its first use.
- L170: need to provide some information about your coordinate system before you say things like the "x and y directions."
- L205: GDM not defined
- Eq 1 is missing a plus sign
- Figure 2 needs a legend for the x's and the red dashed line.
- L297: a more precise definition of POD should be used. It looks like there is a repeated sentence here as well.
- Your definition of localization accuracy (LA) is more commonly referred to as "positive predictive value" or "precision." It might be better to use these more common phrases.
- In the FNF equation, it is not clear what the n_c refers to. It would be better to write out exactly how n_c is calculated (e.g., n_tp + n_fn), as is done with the other equations.