Egusphere-2025-6386 – reply to RC1

(Annika Vogel et al.)

We thank the reviewer for his comments on the manuscript. We provide point-by-point replies (blue) to the reviewers comments (black) below.

As a general reply, we fully agree that detailed evaluation and validation is required to investigate the overall improvements (and degradations) of this new approach. However, we believe that this is beyond the objective and out of the scope of this study. This work focuses on the development steps from theoretical derivations to the implementation, which already includes lots of novel content on the theory. Therefore, we decided to provide only an exemplary demonstration of how such a setup might impact the actual analysis (increments). Longer, more comprehensive evaluation of multiple case studies and comparison with independent information like satellite retrievals will be performed in future as a follow-up study, and produced as routine operational evaluation documentation.
This was mentioned at some locations in the manuscript (e.g. introduction of Sec. 4 and discussion in Sec.5), however we understand that we did not make this clear enough in the general parts of the manuscript. We decided to reformulate the title to stress the focus on theoretical work on parametric uncertainty forecasts, it now reads:

- *"Formulation of parametric uncertainty forecasts towards operational wildfire smoke assimilation"*

We also revised the abstract, introduction (Sec.2) and conclusions (Sec.5) accordingly and checked with rest of the document for consistency. The most important changes now read:

- ***[abstract, new l.2-6]:*** *"This study exploits parametric uncertainty forecasts (PUF) as a computationally efficient alternative to existing ensemble approaches, where the dynamics of error parameters (such as error standard deviations) are explicitly evolved numerically at a fraction of the cost of ensemble-based methods. It focuses on (1) the theoretical derivation of forecast dynamics tailored to near-surface air quality applications with uncertain emissions, and (2) the implementation of PM2.5 forecast error standard deviation into the Canadian air quality model GEM-MACH."*
- ***[abstract, new l.11-12]:*** *"For illustration purposes, the presented formulation is used for assimilation of surface PM2.5 in an exemplary wildfire case study in eastern Canada in July 2023."*
- ***[abstract, new l.17-18]:*** *"The presented work leads the way towards efficient operational assimilation for wildfire smoke and other uncertain air quality events using a parametric Kalman Filter (PKF)."*
- ***[introduction, new l.85-88]:*** *"This parametric approach has been developed for Kalman filter-based data assimilation, where the so-called Parametric Kalman Filter (PKF) includes the equations for the change of the error parameters during the analysis and forecast step. The PKF forecast step is provided by a parametric uncertainty forecast (PUF) whose explicit derivation of prognostic equations of error parameters provides unique insights into the specific forecast error dynamics in the system."*
- ***[introduction, new l.108-109]:*** *"For illustration purposes, the formulation is used in Sec. 4 for assimilation of surface PM2.5 in an exemplary wildfire case study in eastern Canada in July 2023."*
- ***[conclusions, new l.485]:*** *"This study provides a simple parametric uncertainty forecast (PUF) specifically tailored to …"*
- ***[conclusions, new l.491-493]:*** *"This study focuses on (1) the theoretical derivation and investigation of forecast dynamics specific to the requirements of near-surface air quality applications under uncertain emissions, and (2) the setup and implementation of PM2.5 forecast error standard deviation into the GEM-MACH modeling system."*

This manuscript developed a series of theoretical derivation for background error standard deviation (BESD) from processes including advection, vertical diffusion, point emission etc. These dynamic BESD has case-dependent and anisotropic features. There are two major issues in this manuscript. The theoretical derivation used some assumptions, like “assuming concentration errors at emission locations to be highly correlated to local emission errors” (line 661). This assumed condition is usually valid only for short-lived species emitted from isolated point sources, such as SO2 or NOx from power plants. Applying this assumption to wildfire aerosols needs some justifications, considering that PM2.5 aerosols are relatively long-lived species and the impact of upstream emissions could be significant, especial for the forest fires where the fire spots are usually adjacent. Other important factors, such as fire plume rises, were not mentioned. The changed BESD should also affect the assimilation in elevated layers, but this study and discussion are limited in surface PM2.5 only, without touching anything about aerosol optical depth, an important wildfire plume indicator. Another issue is that this manuscript lacks observation-based verification, and study period is too short. The case study application (section 4) only shows the one-day BESD and analysis increment (June 06, 2023), compared with the operational setup. There is no evaluation using observations.

We identified three main aspects in this general comment that we will reply to individually in the following:

A) Assumption that emission errors are highly correlated to local concentration errors:

The reviewer is right in his comment that this assumption was not sufficiently described. In fact, our formulation was misleading: The emission-concentration correlation was not assumed to be equal to one, but we rather approximate a joint parameter denoted as “correlated emission error standard deviation” $\sigma^{\xi}_{E}(x,t) := \sigma_E(x,t) * \rho_{E,\xi}(x,t)$ which consists of the emission error standard deviation and its correlation to the concentration error.

We clarified the derivation in Apx.A6 and in Sec.2.3 which now read:

- ***[Apx.A6, l.690-698]****: “Gives:*

  $$\partial_t V_\xi(x,t) = 2\sigma_\xi(x,t) * \sigma_E(x,t) * \overline{\widetilde{\epsilon_\xi}(x,t) * \widetilde{\epsilon_E}(x,t)} = 2\sigma_\xi(x,t) * \sigma_E(x,t) * \rho_{E,\xi}(x,t) \quad (A33)$$

  Similarly, the change of concentration error standard deviation due to uncertain emissions is given by:

  $$\partial_t \sigma_\xi(x,t) = \frac{1}{\sigma_\xi(x,t)} \overline{\epsilon_\xi(x,t) * \partial_t \epsilon_\xi(x,t)} = \frac{1}{\sigma_\xi(x,t)} \overline{\epsilon_\xi(x,t) * \epsilon_E(x,t)}$$
  $$. = \sigma_E(x,t) * \overline{\widetilde{\epsilon_\xi}(x,t) * \widetilde{\epsilon_E}(x,t)} = \sigma_E(x,t) * \rho_{E,\xi}(x,t) \quad (A34)$$

  Since the emission error standard deviation $\sigma_E(x,t)$ and its correlation to concentration errors $\rho_{E,\xi}(x,t)$ are both unknown external parameters, they are jointly treated as correlated emission error standard deviation w.r.t. the current concentration error in the following:

  $$\sigma^{\xi}_{E}(x,t) := \sigma_E(x,t) * \rho_{E,\xi}(x,t) \quad (A35)”$$

Please note that there is no assumption made up to this point, but rather a reformulation.

Additionally, we added a paragraph to Apx.A6 which shows the connection of the emission-concentration correlation $\rho_{E,\xi}(x,t)$ to the temporal correlation of emission errors **[Apx.A6, l.708-728].** This formulation also shows that adjacent fire hotspots do not affect error variance or standard deviation. This would however become important when spatial error correlation lengths are included as prognostic parameters (compare e.g. Pannekoucke et al., 2016) which is not part of this study.

The description in the main text was corrected accordingly:

- ***[Sec.2.3, l.233-238]****: "The general change of concentration error variance due to point emissions derived in Apx. A6.1 is given by:*

  $$\partial_t V_\xi(x,t) = 2\sigma_\xi(x,t) * \sigma_E(x,t) * \rho_{E,\xi}(x,t) = 2\sigma_\xi(x,t) * \sigma_E^\xi(x,t) \quad (15)$$

  And similarly, for the concentration error standard deviation:

  $$\partial_t \sigma_\xi(x,t) = \sigma_E(x,t) * \rho_{E,\xi}(x,t) = \sigma_E^\xi(x,t) \quad (16)$$

  were $\sigma_E^\xi(x,t)$ denotes the correlated emission error standard deviation w.r.t. the current concentration error. The derivation of the emission equations Eq. (14)-(16) is given in Apx. A6.

  It shows that the emission process can only increase concentration error standard deviation or variance, but only if the emissions are considered to be uncertain and correlated to the current concentration error."

The reason for defining a single joint parameter is that both individual parameters are unknown and detailed analysis would be required to estimate each of them sufficiently (which is left for future work). Instead, this study applies a simple statistical relationship between emission state and this joint unknown parameter. This was described in the theory:

- ***[Sec.2.3, l.249-254]:*** *"For real-case application, both external parameters (emission error standard deviation and emission-concentration error correlation) in Eq. (16)-(15), remain unknown. Each of them is highly difficult to estimate and can be expected to have complex spatio-temporal patterns, particularly for strong case-dependent wildfire emissions. Apx. (A6.2) shows that the emission-concentration correlation is closely related to the temporal correlation of emission errors, which might be further modified by the other dynamical processes. Unless detailed individual estimates are available, the unknown external parameters may be jointly estimated and treated as one model input $\sigma_E^\xi(x,t)$ for the sake of simplicity."*

as well as in the implementation section which now reads:

- ***[Sec.3.2, l.329-335]:*** *"Thirdly, the change of PM2.5 error standard deviation due to uncertain point emissions in Eq. (16) is given by their correlated emission error standard deviation as a joint parameter including the emission error standard deviation and its correlation to the current concentration error. Thus, this joint external parameter is implemented as a single local source term for concentration error similarly to the state emissions as source term for state concentrations. The spatio-temporal field of correlated emission error standard deviations will be treated as point emissions of the respective concentration error standard deviation in the original point emission scheme of the model.*

The critical part of this implementation is the appropriate formulation of the correlated emission error standard deviations which will be discussed below."

- ***[Sec.3.3, l.370-375]:*** *"[…] the linear slope with zero offset is used to estimate the correlated emission error standard deviation (compare Sec. 2.3 and Apx. A6.1):*

  $$\sigma_E^{\xi}(x,t) = \sqrt{V_E^{\xi}(x,t)} \approx \sqrt{\alpha_E} * E(x,t) \quad (20)$$

  where E(x, t) are the spatio-temporal fields of PM2.5 state emissions as sum of the seven aerosol components. Here, the use of the correlated emission error standard deviation as joint input parameter ensures the emission-to-concentration consistency described above."

In the discussion section, we extended the existing statement that the formulation of emission uncertainties is highly simplified and leaves room for improvements using expert knowledge with respect to the correlation-assumption (also in accordance to RC2's major comment 1):

- ***[Sec.5 discussion, new l.510-521]:*** *"In this study, correlated error variances of point emissions w.r.t. concentration errors are assumed to be proportional to local state emissions. Although this proportionality is consistent with the definitions of initial and boundary conditions (emission-concentration consistency), it is a highly simplified assumption of emission error behavior. This joint quantity consists of the emission error standard deviation and its correlation to the current concentration error which are both difficult to estimate and can be expected to have complex spatio-temporal patterns, particularly for strong case-dependent wildfire emissions. Ideally, each component would be individually estimated from detailed analysis studies which are beyond the scope if this work. Concerning the emission error, each preparation step including detection, quantification and vertical distribution of emissions due to plume rise may have itself complex error sources that would need to be considered. It is demonstrated in Apx. (A6.2) that the emission-concentration correlation is closely related to the temporal correlation of emission errors and potentially also to other dynamical processes modifying the error field, whose estimates are still to be investigated in future. Available studies on aerosol layer and plume height comparisons (Griffin et al., 2020) will provide a valuable basis for more sophisticated process-based emission uncertainty estimates."*

- ***[Sec.5 outlook, new l.565-567]:*** *"Concerning the forecast of error standard deviation of PM2.5, there are multiple potential improvements. These include for example improved formulations of error parameters like vertical error correlations and emission errors, including their correlation to concentration errors [...]"*

B) <u>only discussing surface PM2.5:</u>

Indeed, similar to emissions quantification from wildfires, plume rise parameters on wildfire emissions are important variable in all AQ forecast model systems, and both quantities are likely to have uncertainly due to lack of direct measurements combined with large spatiotemporal variabilities on wildfire source, fuel characteristics etc.

In most model applications of wildfire emissions, the evaluation has been focused on surface PM2.5 concentrations that are routinely available and most directly measured. More specifically, for the model system used in this study, the ECCC RAQDPS-FW (Sec. 3.1), is aimed at providing

operational air quality forecast guidance across the country, thus the goal, and emphasis has been on surface PM2.5 (and other air pollutants such as O3, NO2, not emphasized in this study).

This study focuses on the potential improvements in the Canadian operational air quality analysis scheme. As described in the manuscript (old l.270), this scheme currently only considers surface concentrations – elevated layers are not part of the assimilation system yet. Thus, our analysis is restricted to the surface because (1) the operational system is currently not capable to provide analysis of elevated layers, and (2) the reference operational analysis is also only available at the surface which limits our comparison to this layer.

It was already mentioned in description of the current modeling system (Sec.3.1) and the discussion section (Sec.5) that there is a development priority to enable full assimilation cycling for operational air quality in GEM-MACH. This also includes the extension of the analysis to the full 3D state. Without these elevated layers in the analysis scheme, also vertically integrated quantities like AOD cannot be properly investigated.

We formulated this constrain more clearly when describing the current modeling system, introducing the case study and added a related statement on current developments in the discussion:

- ***[Sec.3.1 current modeling system, new l.285-287]:*** *"The setup of the new parametric error forecast presented in this study is compared to the operational setup for air quality analysis at ECCC. Currently, an hourly surface analysis is performed for selected species including PM2.5, which also restricts the analysis and comparison of this study to the surface layer."*
- ***[Sec.4.1 case study description and model setup, new l.410]:*** *"Note that the OAv2 suite only performs hourly surface analyses, with no feedback back into the next forecast."*
- ***[discussion, new l.558-561]:*** *"The general technical implementation of a full assimilation cycling in GEM-MACH is currently a development priority for research as well as operational purposes. In this context, extension of the surface analysis scheme to the full 3D space is required which will also enable comprehensive evaluation of elevated plumes with satellite-based observations."*

C) observation-based verification and study period too short:

This point refers to the general reply (see beginning for a detailed answer) and is actually related to the point above. Of course, verification with independent observations is key for investigating performance of the novel method. However, such an investigation would be based on full assimilation cycling to evaluate the performance of the subsequent forecast, particularly for this case-study where available observations are sparse. We did some experiments where we left out some observations and found that this significantly impact the analysis itself. We concluded that sufficient verification can only be done in full assimilation cycling which is not yet available.

Additionally, we decided to perform a detailed verification and application to more cases in a separate study (mentioned in old l.529f) because this study already includes a lot of novel content. In this study, we intend to focus on the development steps from theoretical derivations to the implementation, and therefor only provide an exemplary demonstration of how such a setup might impact the actual analysis (increments).

Here are some specific comments.

Section 2.1. For the advection of error field, how to consider the wind field error? This derivation assumes no error on meteorological field. However, in real situation, this error should exist.

We agree with the reviewer that uncertainties in the wind field may be an important source of uncertainty. There has been some studies looking into related errors (e.g. Polavarapu et al., 2016). Yet, operational centers do currently not explicitly consider wind field uncertainties in their operational forecasts and assimilation systems (eg CAMS regional forecasts, Colette et al., 2025). Here, the consideration of dynamically-induced uncertainties in the parametric prognostic approach is not straight forward. Compared to well-established ensemble approaches, the theoretical developments of parametric uncertainty propagation are much less understood so far. There has been some initial work on the implementation of wind uncertainties (by Olivier Pannekoucke et al., personal communication, not published yet), but further work is needed before this could be reliably implemented and applied in a operational system. Yet, further work in this direction is planned for the future.

At the current state, uncertainties due to wind cannot be considered in this study. The discussion of the importance to consider this in future work was extended and now reads as follows:

- ***[Conclusions, new l.568-570]:*** "Concentration uncertainties due to wind might become particularly important for wildfires because their usual alignment with streamlines might not be applicable during such rapidly developing events. "

Please also refer to the purpose of this study, which intends to provide a first formulation which represents case-dependent uncertainties better than the current statistical approach, rather than providing a perfect parametric uncertainty forecast. Therefore, we conclude that this aspect is beyond the scope of this study.

Polavarapu, S. M., Neish, M., Tanguay, M., Girard, C., de Grandpré, J., Semeniuk, K., Gravel, S., Ren, S., Roche, S., Chan, D., and Strong, K.: Greenhouse gas simulations with a coupled meteorological and transport model: the predictability of CO_2, Atmos. Chem. Phys., 16, 12005–12038, https://doi.org/10.5194/acp-16-12005-2016, 2016.

Section 2.2 The vertical diffusion of errors only consider the simplest K-theory diffusion. For big wildfire, the plume rise and convection could be the major factor affecting the pollutant's vertical distribution.

We agree that these processes are expected to have a big influence on the uncertainty forecast. However, the presented formulation of processes is limited to the processes applied to state concentrations in GEMMACH. In GEMMACH, plume rise is treated within the preprocessing of fire point emissions. Thus, it is implicitly assumed to be captured by the source term of uncertainties from emissions. We are well aware that the current formulation of this emission uncertainty source term is highly simplified and this preprocessing is actually one of the main aspects where we see large potential for improvements in future (mentioned in the discussion). In future, we envision an improved formulation where process-based uncertainties can be estimated from individual sources, e.g. originating from the plume rise formulation. Prior validation and comparison studies will provide a valuable basis for these process-based emission uncertainty estimates: These include aerosol layer and plume height comparisons (Griffin et al., 2020), CO and NO2 emission quantification and method comparisons (Griffin et al., 2021, 2024), and more

recently, column PM2.5 and chemical compositions (Flood et al, 2025) and fire CO emission inversion comparisons with satellite measurements (Voshtani et al., 2025).

We extended the related descriptions to formulate this more clearly in the manuscript:

- ***[Sec.2, new l.142]:*** *"Note that vertical distribution due to plume rise is already accounted in the pre-processing of fire point emissions and thus not considered as additional process."*
- ***[Sec.2.3 point emissions, new l.222-223]:*** *"Point sources, including wildfires, are pre-calculated for each gridbox, including vertical distribution due to plume rise, and added to the respective concentrations as individual process."*
- ***[Sec.5 Discussion, see corrections for aspect A) of general comment above, new l.510-521]***

Concerning convection: We assume that the reviewer refers to convection arising from the thermal energy of the fires. This feedback process to the dynamics is not yet considered in the GEMMACH model and therefore cannot be considered in the uncertainty forecast at this point.

Section 2.3 As the wildfire spots are usually adjacent, the simple assumption of local emission determining local PM2.5 concentrations could have issues.

See aspect A) of general comment above.

Section 3.1 Insufficient detail on model configuration (e.g., resolution, chemistry scheme, boundary conditions, emissions treatment).

We extended the model description as follows:

- ***[Sec.3.1, new l.259-279]:*** "The meteorology-air quality model GEM-MACH (Global Environmental Multiscale - Modeling Air quality and CHemistry) is developed and operationally maintained at Environment and Climate Change Canada (ECCC). The model is part of the department's operational Regional Air Quality Deterministic Prediction System with Near-Real-Time Wildfire Emissions (RAQDPS-FW). It aimed to provide forecast guidance of criteria ambient air pollutants O3, NO2, and fine and coarse, particulate matters (PM2.5, PM10). Much of the science, technical details and forecast validations of the modeling system are available elsewhere (ECCC 2024a, Morane et al., 2025a, 2025b and references therein) only a short summary is provided.

  GEM-MACH is the core chemical transport model with detailed gas-phase chemical mechanism (ADOM with 46 species and 114 reactions) and the Canadian Aerosol Module (CAM) with 2-bin aerosol-size (PM2.5, PM10) and composition-resolved (sulfate, nitrate, ammonium, elemental carbon, primary and secondary organic matter, crustal material, sea-salt) aerosol species. The model accounts for key chemical processes including emissions, chemical transformations, and wet/dry deposition removals.

  The operational RAQDPS-FW configuration is a one-way coupling of meteorology and chemical processes, where atmospheric chemical compositions are calculated on-line as part of numerical weather prediction, but do not influence, or feedback, the forecast weather processes. The model domain is at 10-km grid covering north American continent and 84-vertical layers in hybrid coordinates from the surface to 0.1hPa. The system simulates the evolution of gas-phase and aerosol chemical species with hourly input of anthropogenic, biogenic and wildfire emissions over the model domain to produce hourly chemical

forecasts for the next 72 hours. Near-real-time wildfire emissions is estimated with the Canadian Forest Fire Emissions Prediction System (CFFEPS) and daily satellite-driven fire locations, and hourly forecast meteorology (Chen et al., 2019). Climatology chemical boundary conditions were adopted from monthly-averaged Community Atmosphere Model with chemistry (CAM-chem) within the Community Earth System model (Tilmes et al., 2022) while hourly meteorology boundary conditions were from the operational Global Deterministic Prediction System (GDPS, ECCC 2024b)."

Moran, M. D., Savic-Jovcic, V., Stroud, C. A., Ménard, S., Gong, W., Zhang, J., Zheng, Q., Chen, J., Akingunola, A., Lupu, A., Menelaou, K., and Munoz-Alpizar, R.: Operational chemical weather forecasting with the ECCC online Regional Air Quality Deterministic Prediction System version 023 (RAQDPS023) – Part 1: System description, EGUsphere [preprint], https://doi.org/10.5194/egusphere-2025-4323, 2025.

Moran, M. D., Lupu, A., Savic-Jovcic, V., Zhang, J., Zheng, Q., Boutzis, E. I., Mashayekhi, R., Stroud, C. A., Ménard, S., Chen, J., Menelaou, K., Munoz-Alpizar, R., Kornic, D., and Manseau, P. M.: Operational chemical weather forecasting with the ECCC online Regional Air Quality Deterministic Prediction System version 023 (RAQDPS023) – Part 2: Multi-year prospective and retrospective performance evaluation, EGUsphere [preprint], https://doi.org/10.5194/egusphere-2025-4324, 2025.

ECCC, 2024a. The Regional Air Quality Deterministic Prediction System (RAQDPS) of the Meteorological Service of Canada, Technical Specifications available from https://collaboration.cmc.ec.gc.ca/cmc/CMOI/product_guide/docs/tech_notes/technote_raqdps_e.pdf

ECCC, 2024b. The Global Deterministic Prediction System G0 (GDPS) of the Meteorological Service of Canada, Technical Specifications available from https://collaboration.cmc.ec.gc.ca/cmc/CMOI/product_guide/docs/tech_notes/technote_gdsps_e.pdf

Tilmes, S., Emmons, L.K., Buchholz, R.R. & The CESM2 Development Team, (2022). CESM2.2/CAM-chem Output for Boundary Conditions. UCAR/NCAR - Atmospheric Chemistry Observations and Modeling Laboratory, DOI: https://doi.org/10.5065/XS0R-QE86.

Chen, J., Anderson, K., Pavlovic, R., Moran, M. D., Englefield, P., Thompson, D. K., Munoz-Alpizar, R., and Landry, H.: The FireWorkv2.0 air quality forecast system with biomass burning emissions from the Canadian Forest Fire Emissions Prediction System v2.03, 770 Geoscientific Model Development, 12, 3283–3310, https://doi.org/10.5194/gmd-12-3283-2019, 2019.

Section 4. The case study is only limited to one-day event, and there is no direct evaluation against observations.

See aspect C) of general comment above.