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Comment on acp-2022-77

Anonymous Referee #1

Referee comment on "Toward targeted observations of the meteorological initial state for improving the PM_{2.5} forecast of a heavy haze event that occurred in the Beijing–Tianjin–Hebei region " by Lichao Yang et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2022-77-RC1>, 2022

The authors study the optimization of observation locations (targeted observation) to achieve an improved forecast for particulate matter. Interestingly they provide an example of a severe haze event in the Beijing area where early warnings by the authorities failed to be timely issued. This topic has attracted interest since more than a decade ago, in recent years also in the realm of atmospheric chemistry. It is strongly linked with research on predictability, observability and data assimilation. A wealth of methods has been devised, or derived from existing techniques found in the aforementioned realms.

In their study "Toward target observations of the meteorological initial state for improving the PM_{2.5} forecast of a heavy haze event that occurred in the Beijing-Tianjin-Hebei region" by Yang Lichao, Duan Wansuo, Wang Zifa, and Yang Wenyi addressed the optimisation of measurement deployment for full and atmospheric chemistry application by devising a meteorological problem of optimal measurement dislocation. In my review I question this strategy with some detail, encouraging the authors to refute my demurs.

Methodology:

The motivation of the work where's to improved aerosol forecast which failed significantly in the case study selected not fault booked. So, there might be different reasons for this failure notably a faulty emission inventory or degraded weather forecasts. In their approach the authors seeked the reason only in the weather forecast. Hence, they tried to improve the prediction by better located meta oral meteorological observations which they assimilated to obtain better initial values for the forecast. The other option let the forecast deficiencies might result from faulty emission inventories was not considered is out giving any evidence of reason. The authors quite deliberately declared a better forecast resulting

from era 5 reanalyses to be the truth while another one from GSE was declared control which verse aspired to be improved by additional and optimally located observations. The resulting simulation product provided the improved forecast in relation to the control room but not as good as the truth run identity fight before. The statistical analyses of the assimilation run were then provided as quantitative proof of concept.

My critique addresses several items.

Firstly, how would the method provide reasonable results if not the meteorological forecasts are deficient but the emission inventory, which are in fact often poorly known. Figure 1 of the manuscript does not give any indication that the major discrepancy is only due to meteorological prediction flaws. In addition, if both forecasts, that is the truth and the control run, suffer from the same problem, as for example poor boundary layer height simulations, then the method proposed incapable to give any evidence of any source of error.

Secondly, I put the assimilation procedure in question. So let us assume the authors are right in their suspicion, that the meteorological forecast is the source of misprediction of the aerosol concentrations. A sound synoptic description of the weather situation and its evolution is lacking as are appropriate surface weather charts. In addition, a discussion on the boundary heights and stability would be in place, as these are a critical parameters, controlling the capture of emissions. What happens, if both truths run and control run err with the stability in the same way, but differ in , say, as in this paper, in the horizontal wind direction? In this case, the CNOP type error is critically incomplete. The method proposed by the authors is designed to deploy 15 different observation locations which might be the key to the sufficiently well performing forecast. So, all in all they select 15 times four height levels times 4 meteorological parameters that means individual 240 observations and tested the performance of these idealised network with respect to varied distances. In fact this is a variable the radiosonde network or air borne drop sonde area placed windward of the area of interest to be predicted. Leaving aside the practicability, I put into question the benefit for improved forecast with 3D-var by localized observations, given the synoptic balance conditions to be fulfilled. The authors result indicates this: Looking at Fig. 9, panels a) and b), it appears to be likely that the eastern side of a high pressure system (northerly winds) at the eastern side of the panels is shifted further eastbound in the truth run (a), than in the control run. It is not possible to correct this error by assimilation of data from a localized observation network alone.

How should the set-up with two model runs operate practically? How do we find the "real truth"? In fact, the only thing what can be done is to achieve an optimal meteorological forecast in general, with all available observations. After this, optimal sensitivity areas can then be identified for chemical concentration measurements, not for meteorological observations, because the truth is not known.

Recommendation: To account for these problems, the authors are encouraged to change their validation strategy and conduct numerical experiments, where the emission inventory is taken as true and a nature run produces artificial ("synthetic") aerosol

concentration observations, which then are to be reproduced by the proposed targeted observation procedure, analog to Observation System Simulation Experiments (OSSE) made in data assimilation developments.

Literature:

The authors claim that they are the first to transfer the method of targeted observation to atmospheric chemistry, which does not at all apply! Regrettably, it appears that the authors are not aware of the number of meanwhile growing set of papers on this very matter. Some relevant papers are given here for convenience. Studies focusing on atmospheric chemistry observation targeting, explicitly or implicitly, are indicated by boldface letters, and merit special attention. As the authors focus on meteorological targeted observations I include several other studies on that issue, which might also be considered.

Recommendation: We strongly recommend who review this literature given below.

Belsky T, Kostelich EJ, Mahalov A (2014) Kalman filter data assimilation: targeting observations and parameter estimation. *Chaos* 24(2):024406.
<https://doi.org/10.1063/1.4871916>

Berliner, L. M., Lu, Z., and Snyder, C.: Statistical design for Adaptive Weather Observations, *J. Atmos. Sci.*, 56, 2536–2552, 1998.

Bishop, C. H. and Toth, Z.: Ensemble Transformation and Adaptive Observations, *J. Atmos. Sci.*, 56, 1748–1765, 1998.

Buizza, R., Cardinali, C., Kelly, G., and Thepaut, J. N.: The value of targeted observations, *ECMWF Newsletter*, 111, 11–20, 2007.

Daescu, D. N. and Carmichael, G. R.: An Adjoint Sensitivity Method for the Adaptive Location of the Observations in Air Quality Modeling, *J. Atmos. Sci.*, 60, 434–450, 2003.

Goris N, Elbern H (2013) Singular vector decomposition for sensitivity analyses of tropospheric chemical scenarios. Atmos Chem Phys 13:5063–5087. <https://doi.org/10.5194/acp-13-5063-2013>

Goris N, Elbern H (2015) Singular vector based targeted observations of chemical constituents: description and first application of EURAD-IM-SVA. Geosci Model Dev 8:3929–3945. <https://doi.org/10.5194/gmd-8-3929-2015>

Khattatov, B. V., Gille, J., Lyjak, L., Brasseur, G., Dvortsov, V., Roche, A., and Waters, J.: Assimilation of photochemically active species and a case analysis of UARS data, J. Geophys. Res., 104, 18715–18738, 1999.

Liao, W., Sandu, A., Carmichael, G. R., and Chai, T.: Singular Vector Analysis for Atmospheric Chemical Transport Models, Mon. Weather Rev., 134, 2443–2465, 2006.

Szunyogh I, Toth Z, Emanuel KA, Bishop CH, Woolen J, Marchok T, Morss R, Snyder C (1999) Ensemble based targeting experiments during FASTEX: the impact of dropsonde data from the Lear jet. Q J R Meteorol Soc 125:3189–3218. <https://doi.org/10.1002/qj.49712556105>

Wu X, Jacob B, Elbern H (2016) Optimal control and observation locations for time-varying systems on a finite-time horizon. SIAM J Control Optim 54(1):291–316. <https://doi.org/10.1137/15M1014759>.

Wu, Xueran; Elbern, Hendrik, Jacob, Birgit; The assessment of potential observability for joint chemical states and emissions in atmospheric modelings, Stochastic Environmental Research and Risk Assessment <https://doi.org/10.1007/s00477-021-02113->, 2022.

The paper is in fact about an algorithm for targeted observations. As such no results for atmospheric chemistry per se are offered and can be expected. So it is suggested to submit the manuscript to GMDD rather than ACPD.

Specific remarks:

- The authors should use the term **targeted** observations throughout, as in the paper by Majumdar. (Not target observations. Majumdar made only deviations by grammatical reasons.)
- Discussion of emission inventory uncertainty and other uncertainty sources. There is a well-established corpus of literature addressing uncertainty sources of chemistry transport model, where meteorological uncertainties are only one among others. The authors' decision to solely focus on meteorology needs a sound quantification.
- What is the assumed dominant composition of PM 2.5 matter (mineral dust, secondary anthropogenic, ...) , and is the emission inventory sufficiently resolved by 30 km grid size?
- Why is the targeted observation approach not applied to emission sources? It is well understood that emissions are rarely measurable (eddy covariance towers are a practically unavailable exemption). Yet concentration observations in the vicinity of sources could be exploited instead with some benefit.

Minor issues

Title: The typical term is. **Targeted** observations. It is recommended, to adapt accordingly.

Feedback emissions-meteo around L 545 mentioned, but emission inventory uncertainties poorly addressed.

Fig. 9 Substantial differences between truth and ctrl run. How is this possible? Could be phase error. This renders the assimilation of artificial data critical as this local information is inconsistent with the synoptic situation (imbalance).

As meteo forecast deficits are assumed for PM prediction flaws: Validation against meteo data lacking. Why?

L 39-50: Do the authors claim that this is valid for their study region, or globally? Most studies point at emission strengths uncertainties. More precisely, the uncertainties of predictions must be pondered with forecast time. On short range forecasts today's meteo forecast uncertainties are small, if not extraneous, when compared with both anthropogenic and biogenic emissions. Please discuss this with more scrutiny.

L 71: This is not applicable. See e.g. Goris and Elbern, GMD, 2015.

L 80: "or even become worse". Theoretical justification needed.

L 150: Should be mentioned here that M is WRF and not the CTM, not only at line 172.

L 160: Readers might appreciate a literature reference for the energy norm eq. (3) .

L 177: Readers could be hinted that this is a realisation of the maximisation of an Oseledec operator, to familiarize with operator P. In fact, it is nevertheless a linear optimisation, linearized around the "nonlinear trajectory" of the model run, as the adjoint is used.

L 183: It is pertinent to provide a map of BTH model domain with observation sites here at latest.

Fig, 1 caption : Add time instances AT and DT for discussion below by some tags for convenience.

L 265: Please give a rigorous definition of "CNOP-type error" here, where it is mentioned first! Is it that what has been described in L 297 f?

L368: Do you mean "differences" instead of "bias"?

L 393: On each level (located through the vertical 950, 850, 750 and 500 hPa levels), or only on the most sensitive level? So, are there 15 or 60 observations?

L461 ff: Why is this subsection reasonable, if the algorithm applied is correct, in that it infers optimal conditions? The value of the method is tested against an improvement of an control run, not against climatologically (?) selected other areas. I suggest subsection 4.3 can be omitted.

L 500: How is a decline possible, as the sensitivity is low? It should at least be neutral.

L 543: More precisely, it should be especially assigned to stagnant conditions, where a stable layer caps the boundary layer.

L 560: What is the sign: truth minus control?

L571: But may increase stability. Further, the interpretation of observed PM values must be supported by information of being dry aerosols or with water component included. The discussion presented should be attentive to that. Otherwise the conclusions may be false.

L640: What is the "vertical integer of CNOP-type errors"?

L662-667: What id the novel message of this passage there than the trivially expected?

L 673: "formation of PM2.5": Strictly speaking, a different local temperature and humidity dependent secondary formation of PM2.5 must be understood, with equal gaseous precursor emissions. It appears unlikely to me, that this can substantially explain the differences given in Fig. 1. Please clarify.

L 687: ..."then formulates a theoretical basis to implement practical field campaigns associated

with air quality forecasts". Please indicate where this can be found!

L 697: What does "logistical verification" mean?