Geoscientific Model Development Discussions

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# Comment on gmd-2021-259

Anonymous Referee #2

Referee comment on "A quantitative decoupling analysis (QDA v1.0) method for the assessment of meteorological, emission and chemical contributions to fine particulate pollution" by Junhua Wang et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-259-RC2, 2021

Review comment on gmd-2021-259

General Comments:

The manuscript 'A quantitative decoupling analysis (QDA v1.0) method for the assessment of meteorological, emission and chemical contributions to fine particulate pollution' written by Junhua Wang presented the QDA method as novel way to evaluate meteorology, emission, and chemistry processes involved for the aerosol formation. Although the concept of this method is interesting, I cannot fully understand the description of method itself and therefore go through to result and discussion section well. At the current presentation quality, this manuscript cannot be considered for publication. At this round, I would like to reject this manuscript. Before considering the possible publication, I sincerely request the fundamental amendments. I wish the following major and minor comments will help to revise this manuscript.

Major Comments:

1. The description of QDA and its relation to IPR

The newly developed QDA method is just the using of six accompanying simulations to calculate M, E, and C terms. In this sense, for example, to drive M term, this method seems to be identical to the SAA as described in the introduction. Actually, how to conduct six accompanying simulations is unclear. Under each time-step simulation, how can do the base-model derive each process? The detailed description of M2-M7 is required to understand the QDA method. In addition, without E term, C term cannot be driven due to the absence of precursors. Therefore I guess that EC term inherently connected and it could be hard to be divided. Moreover, on P4, L118, it was stated that "The above QDA method can also be combine with the IPR method to resolve more detailed information…". This statement is confusing to me because this impressed that QDA is just the using of IPR. Under the current presentation quality, it is difficult to understand QDA method and I cannot recognize this method as novel way in modeling analysis.

2. Results and discussion of QDA.

Because the description of QDA is insufficient, I also cannot follow the result and discussion section. Why E term showed same values through analyzed stages? Is this because emissions did not consider temporal variation through analyzed episode? The meteorological field are shown in Fig. 4, but how about the precipitation? Because the term of "wetdep" was 0.00 through stages, I felt that there was no rain. Although this was the severe haze event, without the wet deposition analysis, this episode seems to be not interesting as test case to show the QDA result. As evaluated using NOR and SOR, I like the idea to consider the formation process from the viewpoint of each specie. The result of QDA is now discussed for PM2.5; however, each specie have been evolved as different E and C terms. I would like to strongly recommend to show the same kind of analysis of Figs. 7-9 for each specie. This analysis will offer the insight into C roles on chemical formation during haze episode.

3. The application of QDA.

As found in the abstract, this QDA method could help modelers to understand the each process and find these uncertainties. I have briefly checked the source code of QDA distributed in ZENODO, but I felt that the fortran90 codes seems to be incorporated into the NAQPMS source codes. How can we apply this source code into other models? If the authors claimed that "QDA is a universal tool", the explanation for how to use this QDA method in other models codes should be kindly introduced within this distribution.

Minor Comments:

P2, L42: CMAQ have to be introduced after the definition of CTM (P2, L56). The organization of introduction for second and third paragraphs should be reconsidered.

P2, L41-46: Under this context, IRR should be also carefully introduced. The IRR can be used to define the role of reaction rate, and this will relate C term in this study.

P4, L92-L99 and Eq. 2: How can we treat the second- and third-order partial differential of x1. x2, and x3? Does this represent the nonlinear term of M, E, and C? What stands for them?

P4, L104: For example, higher temperature will relate activated plant, and change the biogenic emissions intensity. Why E to M is unidirectional?

P4, L112-113: As commented in major point 1, how did conduct accompanying simulations at each time step? The detailed description of each scenario should be explained.

P4, L113-115: However, even though each accompanying simulation conducted at each time step, the result is merely derived from the difference (subtraction) from baseline simulation. What was the advantages to embed these accompanying simulations? How about the computational burden? It was not clearly stated here. Therefore, I cannot follow the importance of QDA method as novel way.

P4, L119-120: In case of sulfate, this will be also produced in aqueous-phase oxidation pathways. How this process was incorporated?

P5, Section 2.2: The core mechanisms configured NAQPMS seems to be outdated over 20 years as stated in this section. Despite the recent progress of modeling components, I

cannot follow "… has been widely used in scientific research and air quality prediction practice (Wang et al., 2014) due to its good performance in simulating the emission, meteorological and chemical processes in the atmosphere.". Detailed introductions of research examples are required, because the modeling performance itself will be important to discuss this manuscript.

P5, L132: Typo in "ISORRPIA".

P5, L142: What was this year? It should be defined first here.

P5, L143-144: What was the height of lowermost layer? It should be explicitly stated to consider the modeling performance at surface level.

P5, L145: Was the MEIC also targeted to the analyzed year?

P5, L147: What kind of biomass burning emissions was used? If not used, why?

P5, L149: Confirm the version of MOZART 2.4 or 2.5?

P5, L151: Again, WRF version 3.7 seems to be also outdated. What is the exact reason to use this version to generate meteorological field despite the authors' claim of the importance of meteorology.

P5, L150-152: Does NAQPMS model online-coupled to WRF meteorological field? It was not clarified here.

P6, L171: Need the definition of LST. What is the difference from GMT?

P7. L193-194: Over China, recommendations of modeling standards have been updated (https://acp.copernicus.org/articles/21/2725/2021/), and it is better to use this criteria because this study targeted BTH region.

Figure 5 and 9: Without the explicit information of vertical layer height, this presentation is weak. Please clarify these information on Section 2.2 or 2.3.

Figure 8: The contribution of M and E terms are larger compared to other terms. I would like to recommend to use different scale for them, especially for (e)-(h). Again as I have commented as major comments of 1 and 2, this result impressed me that QDA was just the usage of IPR method. Please clarify this point in introduction and methodology.

Figure 10: Was the vertical axis used log-scale? It seems to be used unusually scaled axis.