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Interactive comment on "Concentration Trajectory Route of Air pollution with an Integrated Lagrangian model (C-TRAIL model v1.0) derived from the Community Multiscale Air Quality Modeling (CMAQ model v5.2)" *by* Arman Pouyaei et al.

Anonymous Referee #1

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Review

The manuscript describes the implementation of the trajectory-grid technique into the popular CMAQ regional air quality model. It demonstrates the use of this upgraded model in simulating transport of CO during the KORUS-AQ campaign, demonstrating that it could be used to identify likely sources of observed pollution.

The paper is fundamentally suitable for GMD, as it describes an interesting new diag-

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Discussion paper

nostic technique for a widely-used model. The trajectory-grid method is interesting, and the integration of a Lagrangian technique into an Eulerian model has the potential to bring valuable new insights into air quality modeling. However, I believe that the authors overstate their conclusions in ways which are not necessarily supported by their work. I also find that the paper lacks some important methodological details. I would therefore recommend that the paper undergo some revisions before being accepted for publication in GMD.

Major comments

My biggest concern is that certain aspects of the method seem to be either incompletely described or just incomplete. In particular:

1) If parcels are spawned in cells with the concentrations of the closest packet, how is this approach mass conservative? Chock et al (2005) did claim that the T-G method is mass conserving, but they point out that this is not the case when diffusion is simulated. Similarly, it is not clear to me how the spawning and pruning processes (lines 105-109) could occur without either incurring mass conservation errors or acting to artificially diffuse the concentration distribution.

2) The approach described is designed with long range transport in mind, but I could not find any description of how convection is treated. Convective transport could significantly change the path taken by an advected air parcel, and is not trivial to simulate in a Lagrangian framework. How is this phenomenon dealt with in this model? I could not see any reference to it in Figure 2.

I disagree with one of the premises of this study. On lines 46-48, it is claimed that back-trajectory modeling for source-receptor estimation is “not widely accepted because it is unable to determine whether an originated air mass is polluted or non-polluted”. Given the widespread use of back-trajectory modeling for this exact purpose, this statement does not seem justified. Furthermore, it seems to neglect that the same issue exists with the C-TRAIL approach, but in reverse. Unless an simulated air mass exactly coincides with the monitor location at the exact time of an observation, one cannot be certain that it contributed to that specific reading.

Line 198 – what does it mean to "reach Seoul" (altitude)? What is the minimum altitude that a packet has to reach to be considered as "reaching" Seoul? This seems important – if the altitude is too great, then air packets which are simply passing over Seoul (and therefore irrelevant to its air quality) will be incorrectly labeled as contributions. Furthermore it would be strange to compare two parcels which arrived at very different heights.

Throughout the paper, it is claimed that the model is "accurate" (line 296), "ideal" (line 302), and "validated" (line 11). However, the main validation is shown in Figure 4, and – unless I have misunderstood – this just shows that the base CMAQ model (since it does not seem that the TG modifications change the behavior of the base model) can reproduce some of the observed behavior. With that in mind:

1) Why does the model seem to consistently underpredict the observed values? I note that the authors do state as much for the DWP and SP, but they also state "very high correlation" during the EPP. While technically true that the index of correlation is higher during EPP than DWP or SP, this seems misleading when the root mean square error is still 68.7 ppbv.

2) Why does the model appear to have a hard minimum concentration of 50 ppbv CO (see figure 4a)?

3) In what sense is the TG approach "validated" here? If no specific validation of the C-TRAIL approach is given (e.g. by comparing to continuous satellite observations), I would recommend that the authors instead simply state that this is a new diagnostic technique for an existing model.

I applaud the authors for bringing up some of the shortcomings of the method in their conclusions (lines 305-306). However, I recommend that they put a more comprehensive discussion of these limitations in the main text.

Minor comments

Line 29 – the words in HYSPLIT should be capitalized (i.e. "Hybrid Single-Particle Lagrangian Integrated Trajectory")

The manuscript contains numerous grammatical errors. This does not affect the quality of the science or whether it should be accepted, but I would recommend that the authors take another pass through to try and improve this.

I noticed that the code is made available only by request. While this is fine, I would encourage the authors to consider making the code more freely available (e.g. on GitHub) unless they are unable to do so because of some specific restriction.

I recommend that the abstract be toned down. Several claims do not seem to be meaningful (e.g. on line 6, how is the Lagrangian output "reliable" or "comprehensive"?) and others are confusing (e.g. I'm not sure what is meant by "real polluted air masses" – line 8).

More generally, I note that the term "real polluted air mass" turns up many times. I suggest this is changed to simply "polluted air mass" given that these are still all simulation results. Even if the pollution was observed at some point, the model is performing a simulation which will include errors.

On lines 309 and 310, the authors call the model "efficient". However, I did not see any quantification of this in the paper. I suggest that this claim is removed. Alternatively the authors could consider giving a specific estimate of the computational overhead associated with C-TRAIL.

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