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Interactive comment on "The Detailed Emissions Scaling, Isolation, and Diagnostic (DESID) module in the Community Multiscale Air Quality (CMAQ) Modeling System version 5.3" *by* Benjamin N. Murphy et al.

Anonymous Referee #2

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General Comments

Polutant emissions are a key input of chemical transport models, and many applications of these models require emissions modifications. The preparation and perturbation of input emissions is thus an important task for the use of chemical transport models, but this task is usually performed using off-line emissions processing systems. The successful use of emissions processing systems such as SMOKE, however, requires a high level of expertise and experience and typically requires time-consuming, very

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detailed work to be performed in which it is easy to make mistakes and hard to track and document the process and the results. In addition, many chemical transport models now also contain in-line calculation of natural emissions that are influenced by hourly meteorology; these in-line emissions are difficult both to track by the user and to modify without code changes.

This paper describes DESID, a new module for the CMAQ chemical transport model. DESID is in essence a versatile but powerful post-processor for off-line emissions processing systems as it enables further manipulation of the emissions fields produced by an emissions processing system. The DESID module has been designed with a very flexible, compact, yet powerful user interface. Its use can save considerable emissions preparation time and reduce computer storage requirements while providing control over different emissions streams, error checking, and useful output documentation as well as optional output of processed emissions files. The authors correctly note that resources are seldom available for "model refactoring and infrastructure development", but this new module is a welcome exception to this usual constraint and it constitutes a significant addition to the well-established CMAQ air quality modeling system. It will likely be adopted quickly and widely by the large CMAQ user community.

I found this to be a well-structured and well-written paper. I recommend its acceptance after minor revision. To this end I have made a number of specific comments and suggestions below that I believe will improve the final version and that I hope the authors will consider.

Specific Comments

1. It is mentioned on page 2 that emissions processing must address temporal allocation, but the time variation of input emissions files and how DESID treats this variation is only mentioned once in the paper, on page 5, line 132, and I am not sure this mention is totally correct. Input emissions are commonly specified for each hour of the day. If the model time step is less than one hour, will DESID still apply the instruction rules

during each model time step as stated. This may be true for online emissions streams, but is it also true for offline emissions streams? A few words about how the DESID emissions module fits into the CMAQ operator sequence would be helpful as well as a mention of the day-to-day variation of offline emissions streams (i.e., day-specific or day-of-week specific and monthly or seasonal variation).

2. It is also mentioned on page 2 that emissions processing must address chemical speciation, but in the discussion of the Emissions Scaling rules and Table 1 in Section 2.2.2, it is not made clear that one of the eight rule fields, "Emission Variable", is not an inventory emission variable but rather is a speciated emission variable output by the emissions processing system.

3. I found the use of examples in Section 2 very helpful for understanding how DESID works. One point that was not clear to me, however, appears in lines 139-141. If two rules apply to the same region, stream, and emission variable, would this result in the second rule modifying the scaling factor of the instruction corresponding to the first rule? That is, can multiple rules sometimes result in a smaller number of instructions?

4. Section 2.2 does not say what is the minimum number of rules required by the DESID ECI. Can it be zero (i.e., no rules), or if not could the minimum number of rules be given in a new table in the Supplement?

5. An important constraint on DESID noted on line 167 is the degree of disaggregation of the emissions streams input by the model. In lines 340-341 the authors note a traditional treatment of emissions with 2 offline gridded and 8 offline point emissions files vs. a much more detailed treatment with 27 offline gridded and 19 offline point emissions files. The authors might consider adding a new table to the Supplement that lists and compares these two sets of emissions streams (with corresponding environment variables?) as an example of a simulation that makes full use of the capabilities of DESID and what this higher level of inventory disaggregation looks like.

6. I am concerned that the use of Regional Definitions, while very intuitive and ap-

pealing, might not always give exactly the expected results when applied to multiple emissions streams. The issue is how to handle grid cells that straddle two or more regions. The authors state on lines 172-173 that the gridded definition of a region should quantify "the fraction of emissions in each model grid cell that is associated with the region", but I would expect that the value of the fraction of emissions for a border grid cell would frequently vary with the emissions stream. For example, consider the spatial distribution of ammonia emissions from on-road motor vehicles for a grid cell straddling the Indiana-Illinois state line, which will depend on road network geometery, vs. ammonia emissions from fertilizer application, which will depend on the distribution of farms. In effect I think applying a Regional Definition is equivalent to applying the same spatial surrogate to all emissions streams. I definitely am not saying that this limitation should preclude the use of Regional Definitions, but if the authors agree with this concern, then it would be worth noting in the manuscript that some uncertainty will inevitably be associated with the apportionment of emissions between neighboring regions due to this issue. This minor caveat is particularly important for policy applications, where different fractional reductions may be under consideration for different jurisdictions but the actual modeled reductions may be slightly different. Also, I expect this relative uncertainty would likely increase as the size of a region decreases (Rhode Island, say, or a smaller city).

Technical Corrections/Suggestions

p. 2, l. 32 Perhaps "... managers in designing programs to improve urban- ..."

p. 2, l. 43 It is not clear here whether "sources" refers to individual facilities or to different source sectors or source types.

p. 3, l. 71 It is noted here that the paper describes the DESID module as it exists in CMAQ version 5.3.2. Should the paper title reflect this version number?

p. 3, l.77 Perhaps "... and online gridded (e.g., biogenic and marine vapors, ..."

p. 4, l. 103 Perhaps "The rest of this section demonstrates ..."

p. 5, 2nd paragraph. Change the order of the third and fourth sentences?

p. 5, l. 149 Should it be "map emissions variables to CMAQ species with differing units"?

p. 6, l. 157 Just to comment that the table name is not given here but a similar description on l. 221 does give the table name.

p. 6, l. 158 Give a reference for SMOKE.

p. 6, l. 169 Most of the input files discussed in this paper are emissions input files. Would it be helpful to insert a modifier in this sentence, such as geographic input file or regional input file?

p. 6, l. 179 "in the input file"

p. 6, l. 182 "regional expanse" – use an alternate term?

p. 8, l. 224 "i.e." –> "e.g."? (there are other emission inventories in the world)

p. 8, l. 228-229 As written there seems to be some confusion between whether the AIRCRAFT stream (one example) or the WILDFIRE stream (second example) is being discussed.

p. 9, l. 257 "aspect" –> "application"?

p. 11, l. 321-332 The first mention of most of this material is here in the Conclusions section. Would it fit better in the Introduction?

References. There are a number of missing references: and Kelly et al. (2019); Lu et al. (2020); Qin et al. (2020); Robinson et al. (2007); USEPA (2019b); Winijkul et al. (2015).

p. 17, Table 1 Related to Specific Comment 3 above, for the definition of the 'a' operator in the "Op" field, would adding the following parenthetical clause provide more clarity: "(which could result in the modification of an existing scaling factor)"? And some of the matching features are listed; for clarity and completeness, you could list all of them here?

p. 23, Table 7 "BNZ" –> "BENZ"?

p. 24, Table 9 Add footnote to define "Acc"?

p. 26, Figure 2, 2nd column, 2nd box from top "Read multiple offline point «gas» emissions;"?

Section S2. This 6-page section seems a bit unnecessary, since so far as I could tell it differs from Section S1 only in the insertion of three lines (l. 371-373). An alternative could be to list just these lines in this section and state where they would be inserted in the Section S1 ECI table.

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