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## *Interactive comment on* "Impact of a new condensed toluene mechanism on air quality model predictions in the US" *by* G. Sarwar et al.

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General comments: The topics covered in this paper are extremely important to the modeling community and regulatory decision makers and meets the criteria required for publication in Geoscientific Model Development Discussions (with minor revisions). Accurately estimating the daily maximum 8-hour ozone concentration using photochemical grid models is extremely important to the regulatory community. This paper presents a new toluene mechanism and presents the impacts on air quality model predictions. The methodology and analysis are scientifically sound. Although this new toluene mechanism does not have significant impacts on ozone and PM2.5 concentrations, does not alter RRFs, and does not increase OPE; the mechanism does provide a more accurate representation of toluene chemistry that does result in slightly improved

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ozone model performance. Minor revisions include additional analyses not presented in the paper and a more detailed discussion of results. Below are a number of specific comments that should be adequately addressed before the paper is accepted for publication.

Response: We appreciate the reviewer thoughtful comments to improve the paper. We have carefully reviewed each comment and revised the paper accordingly.

Specific Comment: Page 2292 – The introduction should include a discussion on the sources of toluene and the relative importance of anthropogenic and biogenic sources of toluene.

Response: We have included a discussion on the sources of toluene emissions and the relative importance of anthropogenic and biogenic sources of toluene. Section 2.3 provides a description of toluene emissions; thus, we have added the description in Section 2.3 rather than in Introduction. Specifically, we have revised section 2.3 as follows:

Toluene is primarily emitted from anthropogenic sources although some studies (Heiden et al., 1999 and White et al., 2009) suggest that biogenic sources can also potentially emit toluene. Anthropogenic toluene sources include industrial processes involving production of toluene, solvent usage, surface coating operations, printing and publishing industries, automotive exhaust emissions, gasoline storage and distribution facilities (USEPA, 1994). Heiden et al. (1999) conducted laboratory and field experiments, and reported the presence of toluene emissions from sunflowers and pine trees. They suggested that plants under stress can emit more toluene emissions than plants without stress. White et al. (2009) recently reported that alfalfa and pine trees can emit toluene emissions and suggested that biogenic sources in northern New England in the US can emit as much as 13% of the total anthropogenic toluene emissions. Toluene emissions from biogenic sources are generally low and not included in biogenic emissions models such as the Biogenic Emissions Inventory System. In this study, we use

the Biogenic Emissions Inventory System (version 3.13) for estimating biogenic emissions (Schwede et al., 2005); as such toluene emissions from biogenic sources are not included.

Anthropogenic emissions are derived from the 2002 National Emissions Inventory (NEI) for the western US and the 2001 NEI for the eastern US. Total toluene emissions in the western US are lower than those in the eastern US. Typical summertime daily toluene emissions in the western US are about 30% of those in the eastern US. Mobile source sector is the major contributor to toluene emissions burden. On-road and non-road mobile sources collectively contribute 44% and 32% of the total toluene emissions in the western US, respectively. Toluene emissions in urban areas are higher than those in rural areas.

Specific Comment: Page 2293, line 20 – The summer model performance statistics are much more important than the winter model performance statistics. Change "For example, CMAQv4.7 predicts O3 with a normalized median bias of 4.0% and a normalized median error of 13%" to "For example, CMAQv4.7 predicts 8-hour maximum O3 with a normalized median bias of 6.9% and a normalized median error of 14.5% in August, 2006".

Response: We have made the suggested change.

Specific Comment: Page 2298, line 10-11 and Page 2311, Figure 6: It is recommended to add a second line to each chart showing the difference between the observed 8-h maximum ozone concentration and the modeled 8-h maximum ozone concentration (using CB05-Base). This would allow the reader understand how important these changes are to model performance at each monitoring site.

Response: Unfortunately, observed ozone concentrations are not available for the gridcells for which these plots are prepared; thus we cannot add a second line to the chart.

Specific Comment: Page 2298, lines 20-22 and Page 2312, Figure 7: It is recom-

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mended to add the mean normalized bias (MNB) as a function of observed ozone. This would allow the reader to see how normalized performance would vary as a function of observed ozone and allow for comparison to EPA's model performance benchmark of +/-15% MNB.

Response: Adding MNB as a function of observed ozone in the same Figure makes it difficult to read. Thus, we have added a separate Figure (Figure 8 - attached) presenting MNB as a function of observed ozone and revised text as follows. Please note that we have renumbered original Figure 8 and 9 as Figure 9 and 10:

Ambient monitoring data from the United States Environmental Protection Agency's Air Quality System are used to evaluate mean bias (MB) and mean normalized bias (MNB) for O3. The median and inter-quartile range of MB and MNB for daily maximum 8-hr O3 for CB05-TU and CB05-Base are presented in Figure 7 and 8, respectively. Predicted daily maximum 8-hr O3 levels with CB05-Base are lower than the observed data in Los Angeles and predictions with CB05-TU improves the MB and MNB at all observed concentrations. In Portland, Seattle, Chicago, New York/New Jersey, and Detroit CB05-TU increases predicted O3 for all observed O3 and decrease MB and MNB at higher observed O3; however, it also marginally increase the MB and MNB at lower observed O3.

Specific Comment: Page 2300, lines 9-11: The sensitivity study looked at doubling toluene emissions with CB05-Base vs. CB05-TU. However, the relevance should be explained. It does not seem likely that toluene emissions will double in the future. In fact, it is more likely that toluene emissions will decrease in the future; therefore a sensitivity study that compares CB05-Base vs. CB05-TU with a 50% reduction in toluene emissions may be more appropriate.

Response: The magnitude of future toluene emissions will depend on the control of emissions as well as future growth due to population and economic activity. We used emissions from the existing emissions inventory which contain large uncertainties; thus

we conducted a sensitivity study with enhanced toluene emissions. We have revised section 3.6 as follows:

Developing a reliable emissions inventory is a resource intensive process. While tremendous improvements have been made in past years, current emissions inventories still contain large uncertainties (Placet et al., 2000; Sawyer et al., 2000; Werner et al., 2005). To evaluate the sensitivity of predicted O3 to increased toluene emissions, two additional simulations were conducted by doubling toluene emissions (2 x toluene emissions obtained using NEI). One simulation was conducted using CB05-Base with enhanced toluene emissions and the other simulation was conducted using CB05-TU with enhanced toluene emissions. Larger increases in O3 occur between the two mechanisms with enhanced toluene emissions than those with normal toluene emissions. For example, CB05-TU increases daily maximum 8-hr O3 by 9 ppbv in Los Angeles with enhanced toluene emissions compared to an increase of 6 ppbv with normal toluene emissions on July 6. Similarly, CB05-TU increases daily maximum 8-hr O3 by 17 ppbv in Chicago with enhanced toluene emissions compared to an increase of 10 ppbv with normal toluene emissions on July 8. Thus, CB05-TU can produce additional O3 compared to those with CB05-Base if greater toluene emissions are present which suggests that the new mechanism can be important in areas with elevated toluene emissions.

Specific Comment: Page 2303, line 10: Change text to read "CB05-TU decreases MB at higher observed O3 concentrations, and increases MB at lower observed O3 concentrations.

Response: We have made the suggested change.

Technical Corrections Specific Comment: Page 2292, line 11 – Change "Sensitivity study suggests. . ." to "A sensitivity study suggests .."

Response: We have made the suggested change.

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Specific Comment: Page 2301, line 9 – Add space between "NO3" and "are". Response: We have made the suggested change.

Interactive comment on Geosci. Model Dev. Discuss., 3, 2291, 2010.



Fig. 1. New Figure 8

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