



**Impact of a new
toluene mechanism
on model predictions**

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Impact of a new condensed toluene mechanism on air quality model predictions in the US

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Abstract

A new condensed toluene mechanism is incorporated into the Community Multiscale Air Quality Modeling system. Model simulations are performed using the CB05 chemical mechanism containing the existing (base) and the new toluene mechanism for the western and eastern US for a summer month. With current estimates of tropospheric emission burden, the new toluene mechanism increases monthly mean daily maximum 8-h ozone by 1.0–3.0 ppbv in Los Angeles, Portland, Seattle, Chicago, Cleveland, northeastern US, and Detroit compared to that with the base toluene chemistry. It reduces model mean bias for ozone at elevated observed ozone mixing ratios. While the new mechanism increases predicted ozone, it does not enhance ozone production efficiency. Sensitivity study suggests that it can further enhance ozone if elevated toluene emissions are present. While changes in total fine particulate mass are small, predictions of in-cloud SOA increase substantially.

1 Introduction

Toluene is an important aromatic compound that can affect ozone (O_3) and secondary organic aerosol (SOA) in the atmosphere. However, there is currently a great deal of uncertainty related to toluene chemistry (Calvert et al., 2002). Different chemical mechanisms use different approximations for toluene reactions that can result in different ozone predictions. For example, Faraji et al. (2008) used the Carbon Bond IV (CB-IV) (Gery et al., 1989) and the Statewide Air Pollution Research Center (SAPRC-99) chemical mechanisms (Carter, 2000) for Houston and reported that O_3 predictions differed by as much as 40 ppbv. The authors attributed the difference in predicted mixing ratios mostly due to the differences in aromatic chemistry in the two mechanisms. Yarwood et al. (2005) extended the CB-IV mechanism into an updated Carbon Bond (CB05) mechanism consisting of 156 chemical reactions involving 52 chemical species. Sarwar et al. (2008) evaluated the impact of the CB05 mechanism on model predictions in the US

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and reported that the use of CB05 increases predicted O_3 compared to those with the CB-IV. Toluene chemistry in CB05 was retained from the CB-IV chemical mechanism. Recently, Whitten et al. (2010) proposed a new condensed toluene mechanism for CB05 mechanism. They performed simulations using the existing CB05 mechanism as well as the new CB05 mechanism containing the new condensed toluene mechanism for 38 environmental chamber experiments involving different combinations of toluene and oxides of nitrogen (NO_x). They used four different performance metrics to compare model predictions with chamber data: maximum O_3 , maximum $\Delta(NO-O_3)$, NO_x crossover time, and cresol concentrations (NO = nitric oxide). The new toluene mechanism provided better results than the existing toluene chemistry in simulating chamber data. This study examines the impact of the new condensed toluene mechanism on air quality model predictions in the US.

2 Methodology

2.1 Model description

The study uses the Community Multiscale Air Quality (CMAQ) modeling system (version 4.7) (Binkowski and Roselle, 2003; Byun and Schere, 2006) to simulate air quality. Evaluations for the CMAQ modeling system have recently been conducted by comparing model predictions to measured ambient pollutants (Eder and Yu, 2006; Appel et al., 2007; Foley et al., 2010). The CMAQ model has considerable skill in simulating O_3 mixing ratios in the atmosphere. For example, CMAQv4.7 predicts O_3 with a normalized median bias of 4.0% and a normalized median error of 13% (Foley et al., 2010). Two modeling domains are used for the study. One domain focuses on the western US and consists of 213×192 horizontal grid-cells while the other domain focuses on the eastern US and consists of 213×188 horizontal grid-cells with a 12-km resolution. Each model contains 14 vertical layers of variable thickness between the surface and 100 mb with a surface layer thickness of approximately 36 m. Model simulations are performed for the eastern US for July 2001 and for the western US for July 2002.

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The CMAQ chemical transport model is configured to use the mass continuity scheme to describe advection processes, the Asymmetric Convective Model Version 2 (ACM2) (Pleim, 2007) to describe vertical diffusion processes, the multiscale method to describe horizontal diffusion processes, and an adaptation of the ACM algorithm for convective cloud mixing. Aqueous chemistry, aerosol processes, and dry/wet deposition are included. The meteorological driver for the CMAQ modeling system is the PSU/NCAR MM5 system (version 3.5) (Grell et al., 1994). Initial and boundary conditions for this study are obtained from CMAQ model results of a larger modeling domain.

Each domain is first simulated using the CB05 chemical mechanism containing existing toluene chemistry (CB05-Base) (Yarwood et al., 2005) and then using the CB05 chemical mechanism containing the new toluene chemistry (CB05-TU) (Whitten et al., 2010). The difference in modeling results obtained with the two model simulations are attributed to the differences in toluene chemistry.

The CMAQ modeling system currently provides three different gas-phase chemistry solvers: the Sparse-Matrix Vectorized Gear Algorithm solver, the Rosenbrock solver, and the Euler Backward Iterative (EBI) solver. The EBI solver is dependent on chemical mechanism which necessitates the development of a new EBI solver for each new mechanism. The Rosenbrock and the Sparse-Matrix Vectorized Gear Algorithm solvers are generalized solvers that can usually be used for any chemical mechanisms without requiring any changes. The Sparse-Matrix Vectorized Gear Algorithm solver is the slowest but the most accurate among the three solvers. The Rosenbrock solver is faster than the Sparse-Matrix Vectorized Gear Algorithm solver and was used for this study. The use of CB05-TU increases computational time of the model by 3–6% compared to the CB05-Base.

2.2 Toluene chemistry

Toluene chemistry in CB05-Base contains 10 chemical reactions involving 5 chemical species. A simplified schematic diagram of the toluene chemistry in CB05-Base is

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presented in Fig. 1. Reaction of toluene (TOL) with hydroxyl radical (OH) proceeds via three different channels: 36% of the reaction produces cresol (CRES), 56% produces a bicyclic peroxy radical (TO2), and 8% produces benzaldehyde. Contribution of benzaldehyde to O₃ is negligible; thus, it is not further retained in CB05. TO2 reacts with nitric oxide (NO) to produce organic nitrate (NTR) and a ring-opening product (OPEN) or breaks down to produce CRES. OPEN reacts with OH to form acetyl peroxy radical (C2O3), which subsequently produces peroxy acetyl nitrate (PAN) via reaction with nitrogen dioxide (NO₂). During daytime, CRES reacts with OH to produce methyl phenoxy radical (CRO), which produces NTR via reaction with NO₂.

Whitten et al. (2010) describe the detailed chemistry of CB05-TU containing 26 chemical reactions involving 13 species for toluene oxidation and provide a simplified schematic diagram for the chemistry (see Fig. 3 in the reference). Reaction of toluene with OH proceeds via four different channels: 18% of the reaction produces CRES, 65% produces TO2, 10% produces benzaldehyde, and 7% produces OH. TO2 reacts with NO to produce NTR, OPEN, and methyl glyoxal. OPEN reacts with OH to form a peroxyacyl radical (OPO3), which leads to an organic PAN (OPAN) via reaction with NO₂. During daytime, CRES reacts with OH to generate CRO, which produces nitro-cresol (CRON) via reaction with NO₂. CRON reacts with OH and leads to an alkoxy radical (CRNO) which further reacts with NO₂ yielding NTR.

The impact of the revised toluene mechanism on photochemistry and O₃ production are best illustrated by the following reactions:



where HO_2 = hydroperoxy radical, RO_2 = organic peroxy radical, and $\text{O}(^3\text{P})$ = oxygen atom (triplet), O_2 = oxygen.

The reaction of NO with HO_2 converts NO into NO_2 and cause an increase in O_3 when NO_2 is photolyzed according to reactions (1)–(3) (Finlayson-Pitts and Pitts, 2000). The reaction of NO with RO_2 also converts NO into NO_2 and causes an increase in O_3 when NO_2 is photolyzed (reaction 4) (Finlayson-Pitts and Pitts, 2000). CB05-TU enhances HO_2 and RO_2 directly as well as indirectly through increase in OH and its subsequent reactions with volatile organic compounds (VOC). If sufficient toluene is present, the new condensed toluene mechanism can enhance HO_2 and RO_2 , and subsequently O_3 . Since CB05-TU enhances OH, it can also affect other pollutants.

2.3 Emissions

Anthropogenic emissions are derived from the 2002 National Emissions Inventory (NEI) for the western US and the 2001 NEI for the eastern US. Biogenic emissions are estimated using the Biogenic Emissions Inventory System (version 3.13) (Schwede et al., 2005). 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 and eastern US, respectively. Toluene emissions in urban areas are higher than those in rural areas.

3 Results and discussion

3.1 Impact on O_3 and selected gaseous species

Predicted monthly mean O_3 with CB05-Base and the percent increase in O_3 between CB05-TU and CB05-Base are shown in Fig. 2. Mean O_3 mixing ratios of greater than 40 ppbv are predicted over most areas in the western and eastern US. CB05-TU

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increases mean O_3 in three large areas in the western US and three large areas in the eastern US by 2% or more: Los Angeles; Portland; Seattle; Chicago and the surrounding area; the Lake Erie area including Detroit, Cleveland, Toronto; and the northeastern US coast. Additionally, it increases mean O_3 by more than 0.5% in some areas in the western US and over a large area in the eastern US. Mean toluene/VOC ratios are also shown in the figure. Toluene/VOC ratios are greater in urban areas than in rural areas. Enhancements in O_3 levels coincided with greater toluene/VOC ratios.

Monthly mean OH, HO_2 , and RO_2 with CB05-Base and the percent increases in mean OH, HO_2 , and RO_2 between the two mechanisms are shown in Fig. 3. Mean OH mixing ratios over 0.1 pptv are predicted in many areas in both domains. CB05-TU increases mean OH by more than 1% in many areas in the eastern US as well as in isolated areas in the western US. Mean HO_2 mixing ratios of over 10.0 pptv are predicted in most areas in western as well as eastern US. CB05-TU increases mean HO_2 by more than 2% in Los Angeles, Portland, Seattle, Chicago and the surrounding area, the Lake Erie and the surrounding area, northeastern US coast, and some other smaller areas. Mean RO_2 mixing ratios over 40 pptv are predicted in large part of the western US as well as southeastern US. CB05-TU increases mean RO_2 by more than 2% in coastal states and some smaller areas in the western US and over large areas in northeastern US and smaller areas in eastern US. Generally, larger changes in mean OH, HO_2 , and RO_2 occur in areas with larger O_3 changes. Enhanced HO_2 and RO_2 increases O_3 via reactions (1)–(4).

Monthly mean NO_x reaction products ($NO_z = NO_y - NO_x$) with CB05-Base and the percent increases in NO_z between CB05-TU and CB05-Base are shown in Fig. 4. Relatively high NO_z values (>3.0 ppbv) are predicted over a large area in the eastern US while such levels are predicted only over scattered areas in the western US. CB05-TU increases NO_z both in the western and eastern US in the same areas that it increases O_3 . The primary reason for the increase in NO_z is daytime nitric acid (HNO_3) production via the reaction: $NO_2 + OH = HNO_3$. CB05-TU enhances OH, thus produces more daytime HNO_3 and increases NO_z .

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3.2 Impact on daily maximum 8-h O₃

Monthly mean daily 8-h maximum O₃ with CB05-Base and increases in mean 8-h O₃ between CB05-TU and CB05-Base are shown in Fig. 5. Elevated levels of 8-h O₃ (>55 ppbv) are predicted over only a small area in the western US while similar levels are predicted over a large area in the eastern US. CB05-TU increases monthly mean 8-h O₃ by a maximum of 2.8 ppbv in Los Angeles, 1.5 ppbv in Portland, 1.5 ppbv in Seattle, 2.0 ppbv in Chicago, 1.9 ppbv in Cleveland, 1.7 ppbv northeastern US, and 1.3 ppbv in Detroit compared to those obtained with the CB05-Base. CB05-TU also increases mean 8-h O₃ by 0.5 ppbv or more in several other areas.

Day-to-day variation of the increases in daily 8-h maximum O₃ for Los Angeles, Portland, Seattle, Chicago, New York, and Detroit is presented in Fig. 6. For each area, changes in daily 8-h maximum O₃ between CB05-TU and CB05-Base vary from day to day. While increases are relatively high (5–10 ppbv) on some days, increases are modest on many other days. In Los Angeles, O₃ increases occur on most days while increases in O₃ in Portland and Seattle occur on fewer days. Increases in Chicago and New York are comparable while increases in Detroit are lower than those in Chicago or New York.

3.3 Comparison with observed data

Ambient monitoring data from the United States Environmental Protection Agency's Air Quality System are used to evaluate mean bias (MB) for O₃. Variations in predicted daily maximum 8-h O₃ and MB (median and inter-quartile range) as a function of observed O₃ for CB05-TU and CB05-Base simulation is presented in Fig. 7. Predicted daily maximum 8-h O₃ levels with CB05-Base are lower than the observed data in Los Angeles and predictions with CB05-TU improves the MB 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 at higher observed O₃; however, it also marginally increase the MB at lower observed O₃.

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3.4 Impact on ozone production efficiency

Ozone production efficiency (OPE) is defined as the number of O_3 molecules formed from each molecule of NO_x oxidized to NO_z and can be calculated from the slope of a regression between O_3 and NO_z . OPE are estimated using O_3 and NO_z values during daytime (10:00–05:00 p.m.) and when O_3/NO_x are greater than 46 (aged air mass) (Arnold et al., 2003). OPE obtained with CB05-TU is marginally lower than the value obtained with CB05-Base at Los Angeles (OPE = 5.9 with CB05-TU and OPE = 6.3 with CB05-Base). OPE obtained with CB05-TU is similar to the value obtained with CB05-Base at Chicago (OPE = 4.1 with both CB05-TU and CB05-Base). Increases in O_3 with the new mechanism are associated with increased NO_z . Similar changes are obtained for other areas in the western and eastern US. Thus, CB05-TU increases O_3 by increasing NO_z and without enhancing OPE.

3.5 Impact on air pollution control strategy

While predicted O_3 mixing ratios are important for model evaluation, relative reduction factors (RRF) are valuable for developing emissions control strategies. To evaluate RRF, additional model simulations were performed with a 25% reduction in NO_x emissions using each mechanism. RRF are calculated using results obtained with normal and reduced NO_x emissions for each mechanism. RRF calculated with CB05-Base are identical to values obtained with CB05-TU for most areas. Only minor changes (0.01–0.02) occur in RRF for some isolated areas. CB05-TU does not change RRF compared to those with CB05-Base; thus it is not expected to affect inferences on air pollution control strategies drawn from the model.

3.6 Sensitivity of predicted O_3 with toluene emissions

To evaluate the sensitivity of predicted O_3 to toluene emissions, two additional simulations were conducted with increased toluene emissions (2× toluene emissions

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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 O_3 occur between the two mechanisms with enhanced toluene emissions than those with normal toluene emissions. For example, CB05-TU increases daily maximum 8-h O_3 by 9 ppbv in Los Angeles with enhanced toluene emissions compared to an increase of 6 ppbv with normal toluene emissions on 6 July. Similarly, CB05-TU increases daily maximum 8-h O_3 by 17 ppbv in Chicago with enhanced toluene emissions compared to an increase of 10 ppbv with normal toluene emissions on 8 July. Thus, CB05-TU can produce additional O_3 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.

3.7 Impact on selected aerosol species

Monthly mean anthropogenic SOA, biogenic SOA, and in-cloud SOA with CB05-Base and their percent increases between the two mechanisms are shown in Fig. 8. Predicted anthropogenic SOA concentrations are greater in eastern US than those in western US. Concentrations over $0.05 \mu\text{g m}^{-3}$ are predicted over most areas in the eastern US while such levels are predicted only over smaller areas in western US. CB05-TU increases anthropogenic SOA by more than 2% in northwestern US, Los Angeles, and northeastern US. Carlton et al. (2010) describes SOA formation mechanisms in CMAQv4.7. In CMAQ, benzene, toluene, and xylene (precursors to anthropogenic SOA) react with OH to produce organic peroxy radicals. These organic peroxy radicals react with NO to produce semi-volatile organic compounds and HO_2 to produce non-volatile SOA. Semi-volatile organic compounds produced via the NO reaction pathway can partition to form SOA. Semi-volatile organic compounds can also form non-volatile oligomers through particle phase-reactions. While the CB05-TU produces more organic peroxy radicals via reactions of VOCs with enhanced OH, increases in SOA via the NO reaction pathway are small since NO also decrease with CB05-TU. Since HO_2 increases with CB05-TU, SOA produced via the HO_2 reaction pathway becomes more important and consequently anthropogenic SOA increases.

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Monthly mean biogenic SOA concentrations exceeding $0.4 \mu\text{g m}^{-3}$ are predicted over the southeastern US while such values are predicted only over a small area covering northern California and southern Oregon. CB05-TU increases biogenic SOA by more than 1.0% over a wide area in the southeastern US while increases in western US are generally lower than 1.0% and occurs only over small areas. In CMAQ, isoprene, monoterpene, and sesquiterpene are precursors to biogenic SOA. For SOA production from isoprene, only reaction with OH is considered. For SOA production from monoterpene, reactions with OH, O_3 , $\text{O}(^3\text{P})$, and NO_3 are considered. For SOA production from sesquiterpene, reactions with OH, O_3 , and NO_3 are considered. These reactions produce semi-volatile organic compounds which partition to form SOA. The semi-volatile organic compounds can also form oligomers through particle phase-reactions. Acid enhanced isoprene SOA is also accounted in the mechanism. Since oxidants increase with CB05-TU, biogenic SOA also increases. Although percent increases in biogenic SOA and anthropogenic SOA are similar, absolute increases of biogenic SOA are much larger.

Monthly mean in-cloud SOA concentrations of greater than $0.2 \mu\text{g m}^{-3}$ are predicted over a large portion of the eastern US while in-cloud SOA concentrations in the western US are generally lower than $0.2 \mu\text{g m}^{-3}$ and are predicted only over small isolated areas. CB05-TU increases in-cloud SOA by more than 12% over much of the northeastern US while it increases in-cloud SOA by more than 12% only over small isolated areas in western US. Aqueous-phase oxidation of glyoxal and methylglyoxal by OH produce in-cloud SOA (Carlton et al., 2008, 2010). Glyoxal is not a chemical species in CB05; therefore only methylglyoxal is used for in-cloud SOA production (Carlton et al., 2010). CB05-TU enhances both methylglyoxal and OH; thus in-cloud SOA increases.

The relative contributions of anthropogenic, biogenic, and in-cloud SOA to total SOA with CB05-TU are compared to those with CB05-Base. The relative contribution of anthropogenic SOA with each mechanism ranges up to 54% in the western US and 39% in the eastern US. The spatial distribution of the relative contribution of anthropogenic SOA is similar with each mechanism in each domain (the largest difference is

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4% in each domain). The relative contribution of biogenic SOA with each mechanism ranges up to 88% in the western US and 80% in the eastern US. The largest difference of the relative contribution of biogenic SOA was 7% in the western and 4% in the eastern US. The highest relative contribution of in-cloud SOA increased from 69% with CB05-Base to 75% with CB05-TU in the western US and from 46% with CB05-Base to 52% with CB05-TU in the eastern US. Thus, the relative contribution of anthropogenic, biogenic, and in-cloud SOA to total SOA did not substantially change between the two mechanisms.

Monthly mean aerosol sulfate, nitrate, ammonium, and total $\text{PM}_{2.5}$ with CB05-Base and their percent increases with CB05-TU are shown in Fig. 9. CB05-Base predicts relatively low aerosol sulfate ($<1.5 \mu\text{g m}^{-3}$) over most of the western US compared to relatively high predictions ($>3.0 \mu\text{g m}^{-3}$) over most of the eastern US. It predicts relatively high aerosol sulfate ($>6.0 \mu\text{g m}^{-3}$) over the Ohio valley area in the eastern US while similar concentrations are not predicted in the western US. Predicted values reach up to $1.5\text{--}4.5 \mu\text{g m}^{-3}$ only over a small area in the western US. CB05-TU increases aerosol sulfate by 0.5–1.5% in small areas in the western US and 0.5–1.0% in small areas in the eastern US.

Predicted mean aerosol nitrate of greater than $0.8 \mu\text{g m}^{-3}$ are predicted only over isolated areas in the western US while similar values are predicted over a much larger area in the eastern US. CB05-TU increases aerosol nitrate by more than 2.0% in some isolated areas in the western and larger areas in the eastern US. CMAQ produces aerosol nitrate from the partitioning of HNO_3 , which is produced via nighttime homogeneous and heterogeneous hydrolysis of dinitrogen pentoxide as well as daytime production via $\text{NO}_2 + \text{OH} = \text{HNO}_3$. The primary reason for the increase in aerosol nitrate is the enhancement of the daytime production of HNO_3 .

Mean ammonium concentrations of greater than $1.2 \mu\text{g m}^{-3}$ are predicted over most of the eastern US while similar concentrations are predicted over only small areas in the western US. CB05-TU increases ammonium over only small isolated areas in both the western and eastern US by 0.5–1.0%. CB05-Base predicts greater than $10.0 \mu\text{g m}^{-3}$

of $PM_{2.5}$ in most areas in the eastern US while concentrations are typically lower than $5.0 \mu\text{g m}^{-3}$ for most of the western US. CB05-TU increases $PM_{2.5}$ by 0.5–2.5% in some areas in the western and 0.5–1.0% in the northeastern US. However, increases over 1.0% occur in only a few isolated areas in the western US where predicted mean $PM_{2.5}$ concentrations are generally lower than $5.0 \mu\text{g m}^{-3}$.

4 Summary

CB05-TU enhances monthly mean daily 8-h maximum O_3 by a maximum of 2.8 ppbv in the western US and 2.0 ppbv in the eastern US. These changes are largely confined to the vicinity of major urban areas. CB05-TU improves MB at higher observed O_3 concentrations. CB05-TU enhances OH, HO_2 , RO_2 , and NO_z levels compared to the CB05-Base. While it enhances O_3 , it does not increase OPE. The use of CB05-TU does not alter RRF; thus, relative to CB05-Base it is not expected to alter inferences on air pollution control strategy. Its impact on $PM_{2.5}$ is small. This study uses relatively coarse horizontal grid spacings since it focuses over a large geographical area. The impact of the new toluene chemistry on air quality modeling results could be more pronounced in areas with higher toluene emissions if finer horizontal grid spacings are used.

Disclaimer. Although this paper has been reviewed by EPA and approved for publication, it does not necessarily reflect EPA's policies or views.

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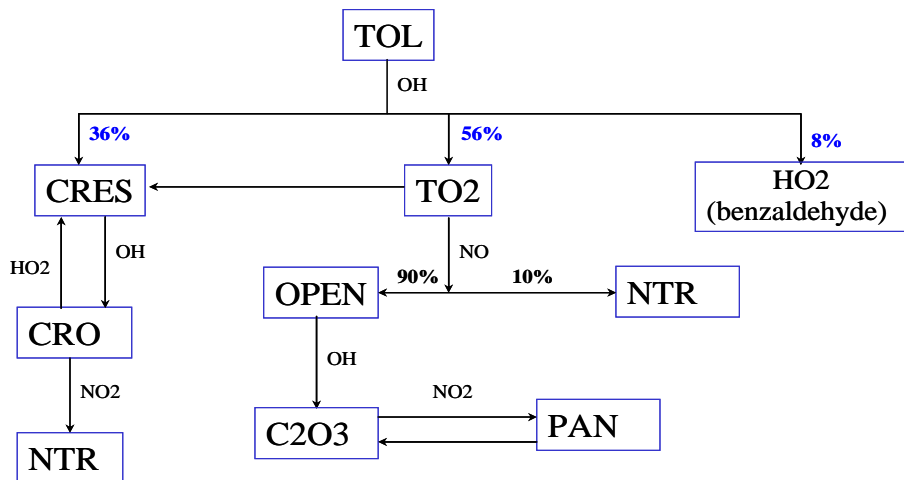
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**Fig. 1.** A simplified schematic diagram of toluene chemistry in CB05-Base mechanism.[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

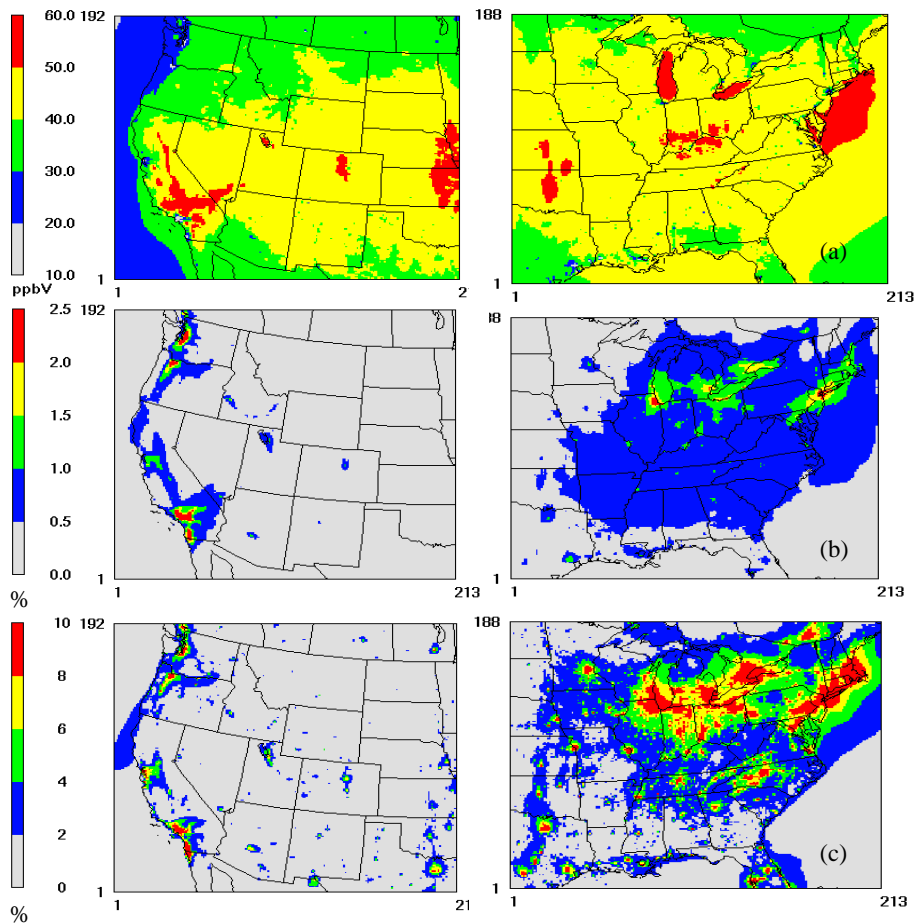


Fig. 2. (a) monthly mean O_3 with CB05-Base, (b) percent increases in mean O_3 between CB05-TU and CB05-Base, (c) toluene/VOC ratio.

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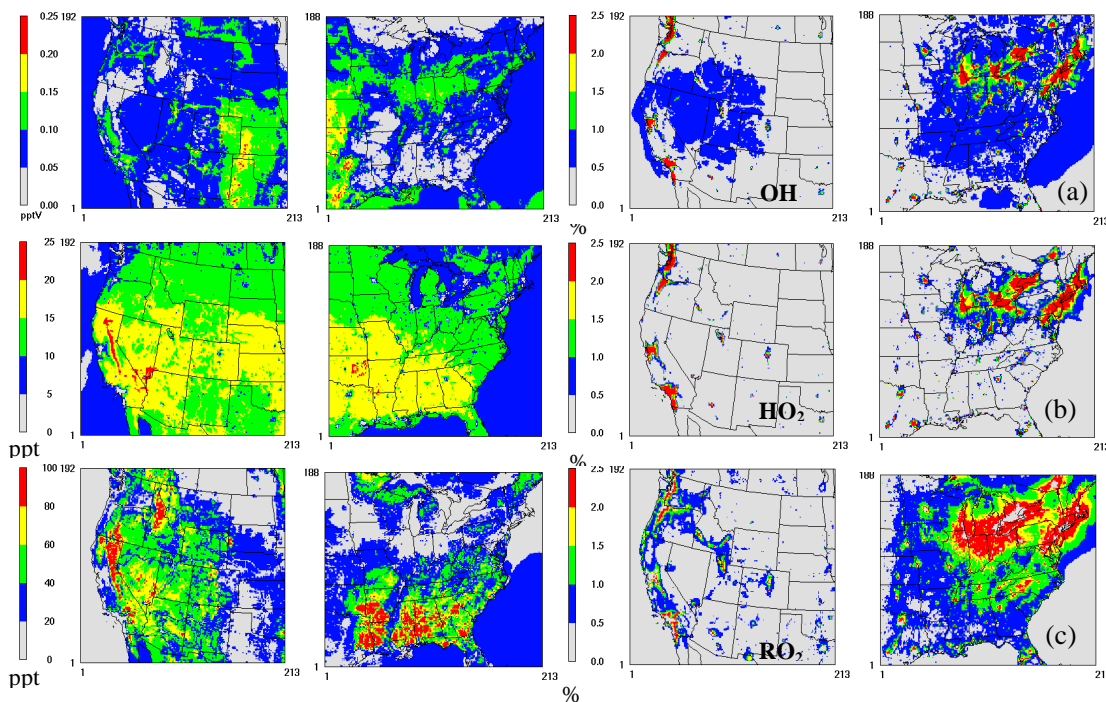


Fig. 3. (a) monthly mean OH with CB05-Base and percent increases in mean OH between CB05-TU and CB05-Base, (b) mean HO₂ with CB05-Base and percent increases in mean HO₂ between CB05-TU and CB05-Base, (c) mean RO₂ with CB05-Base and percent increases in mean RO₂ between CB05-TU and CB05-Base. In each row, the first two plots represent mean values and the last two plots represent percent changes.

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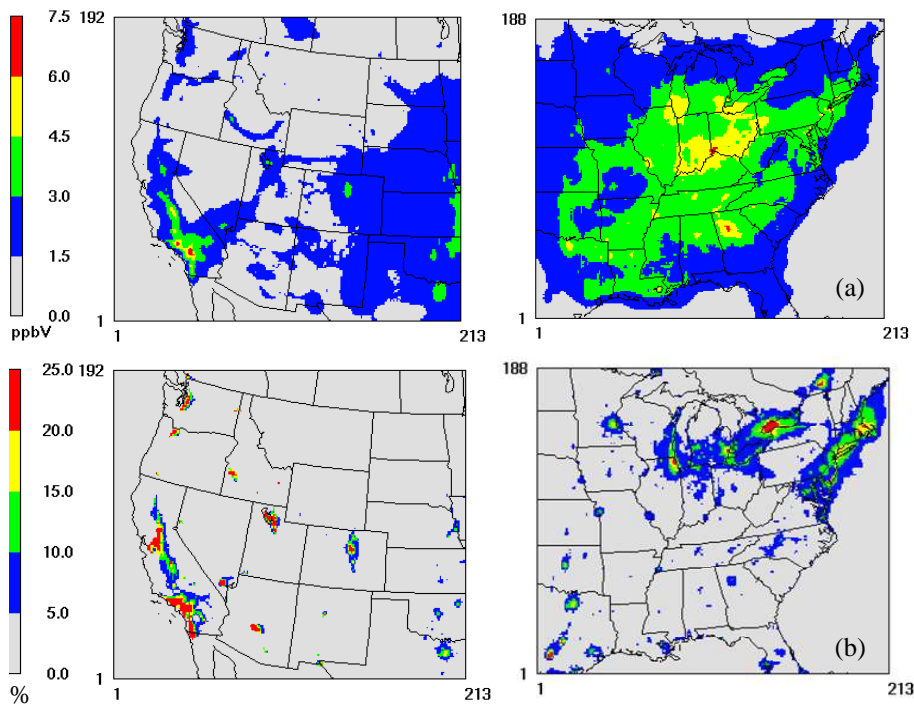


Fig. 4. (a) monthly mean NO₂ with CB05-Base, (b) percent increases in mean NO₂ between CB05-TU and CB05-Base.

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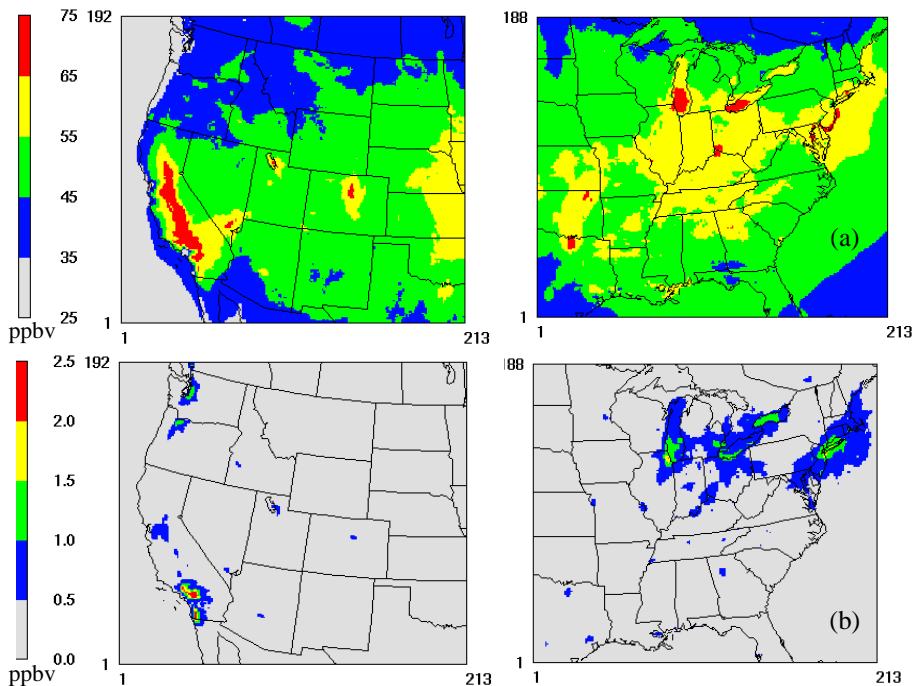


Fig. 5. (a) Monthly mean daily 8-h maximum O₃ with CB05-Base, (b) absolute increases in mean daily 8-h maximum O₃ between CB05-TU and CB05-Base.

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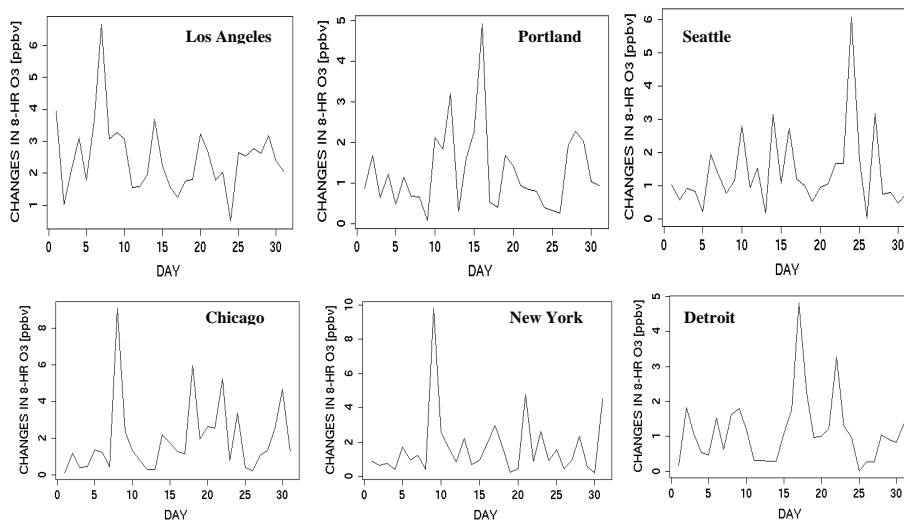
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**Fig. 6.** Day-to-day variation of the increases in daily 8-h maximum O₃ in selected areas.[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

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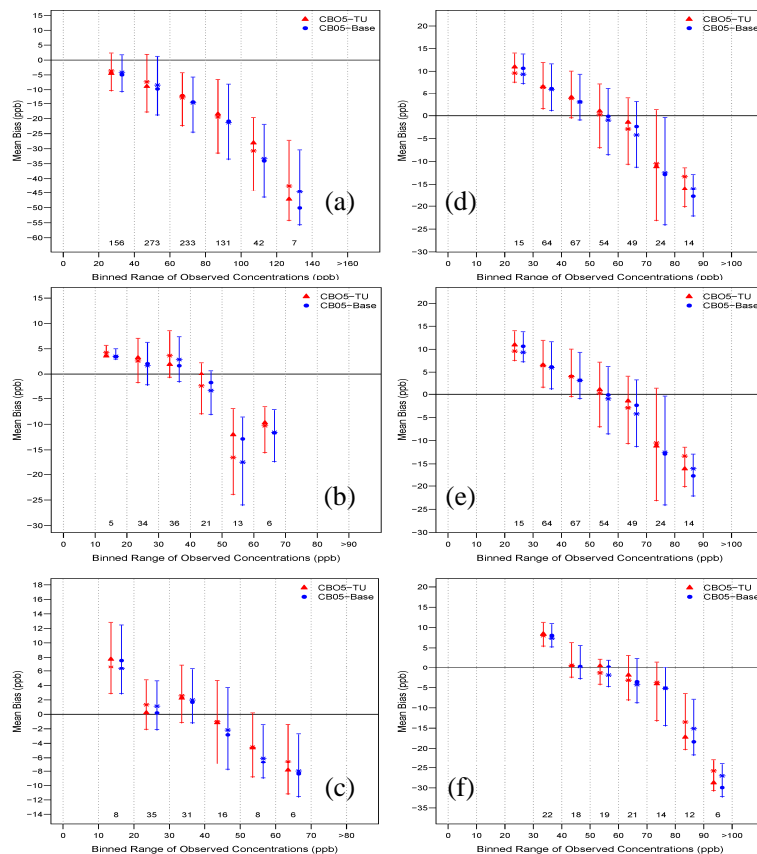


Fig. 7. The median and inter-quartile range of mean bias for the daily maximum 8-h O_3 with CB05-TU and CB05-Base: **(a)** Los Angeles, **(b)** Portland, **(c)** Seattle, **(d)** Chicago, **(e)** New York/New Jersey, **(f)** Detroit. Number beneath each paired evaluation represents the total sample number in each binned range of observed concentration.

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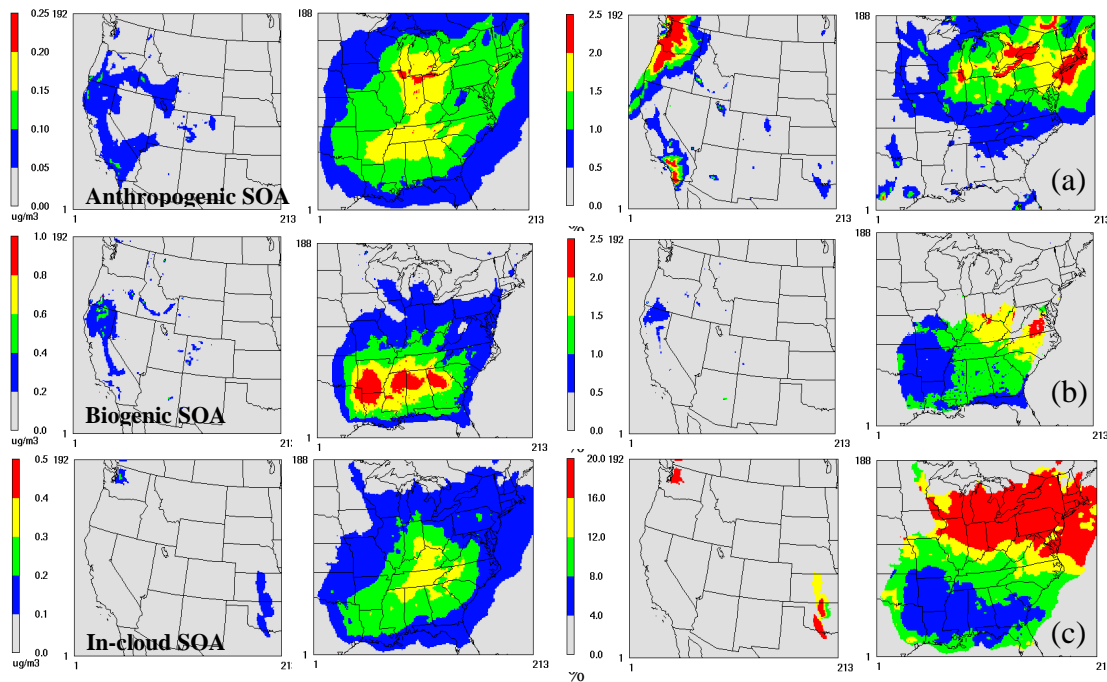


Fig. 8. (a) monthly mean anthropogenic SOA with CB05-Base and percent increases in mean anthropogenic SOA between CB05-TU and CB05-Base, (b) mean biogenic SOA with CB05-Base and percent increases between CB05-TU and CB05-Base, (c) mean in-cloud SOA with CB05-Base and percent increases in mean in-cloud SOA between CB05-TU and CB05-Base. In each row, the first two plots represent mean values and the last two plots represent percent changes.

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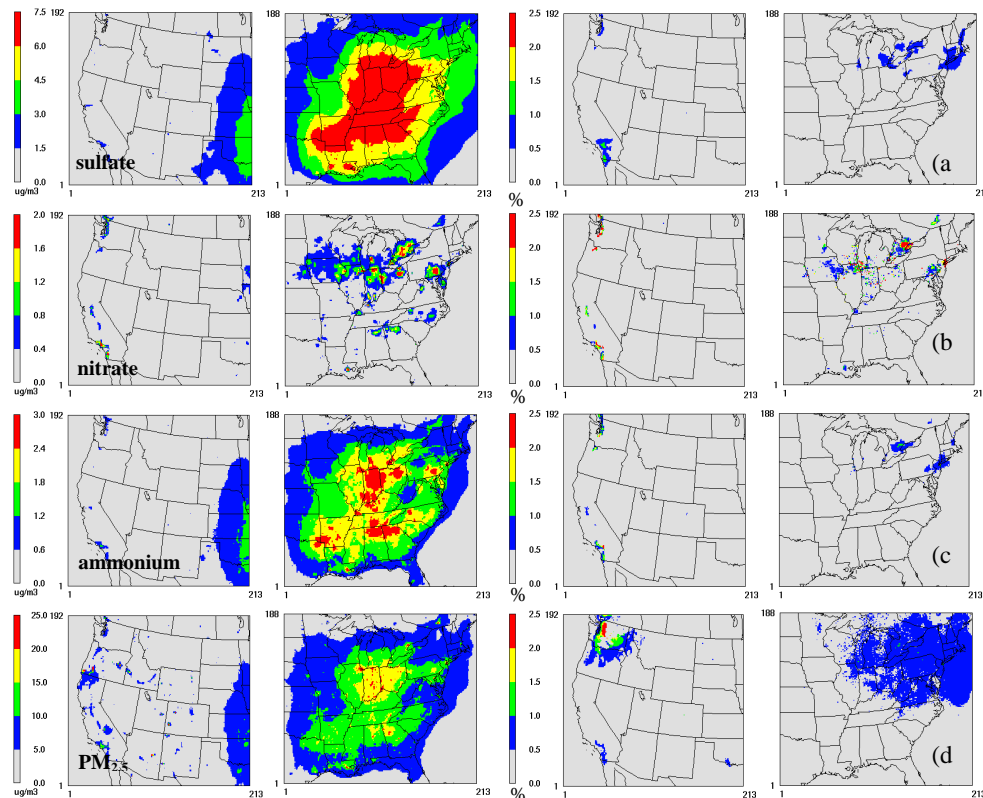


Fig. 9. (a) monthly mean aerosol sulfate with CB05-Base and percent increase in mean aerosol sulfate between CB05-TU and CB05-Base, (b) mean aerosol nitrate with CB05-Base and percent increases in mean aerosol nitrate between CB05-TU and CB05-Base, (c) mean ammonium with CB05-Base and percent increases in mean ammonium between CB05-TU and CB05-Base, (d) mean $PM_{2.5}$ with CB05-Base and percent increases in mean $PM_{2.5}$ between CB05-TU and CB05-Base. In each row, the first two plots represent mean values and the last two plots represent percent changes.

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