Interpreting predictions from the SAPRC07 mechanism based on regional and continental simulations.

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ABSTRACT

The SAPRC07T mechanism is implemented and evaluated in the CMAQ air quality model. The implementation is described and tested with simulations over the United States for two periods. The evaluation compares results against observations for ozone and particulate matter as well as against predictions from the SAPRC-99 mechanism for the same simulation periods and model domains. Comparisons against SAPRC-99 results reveal largest differences over urban areas with low VOC to NO_X ratios. Integrated rate analysis is used to investigate the chemical reactions responsible for these differences. Comparison against observations shows over predictions of ozone concentrations over the southeastern United States. The errors appear linked to failing to match the observations during early morning hours. We discuss the source of the errors in terms of both simulation inputs and the photochemical mechanism and recommend potential directions for improving applications with regional photochemical models.

Key Words: SAPRC, air quality model, tropospheric photochemistry

1. Introduction

Regional Air Quality Models (RAQMs) are being used for developing emission control strategies to decrease pollutant concentrations below harmful levels. One important component of RAQMs is the chemical mechanism, which describes the complex series of chemical reactions

taking place in the atmosphere including the interactions among pollutants. However, there is a major problem when modeling tropospheric chemistry – the number of chemicals and reactions is at least an order of magnitude larger that can be practically simulated in RAQMs, especially at regional-to-global scales. The Master Chemical Mechanism, for example, contains over 13,000 reactions for over 4,000 VOC species (http://mcm.leeds.ac.uk/MCM; Saunders et al., 2003). While there are some examples of complex mechanisms being used in RAQMs, (Jacobson and Ginnebaugh, 2010; Ying, 2011), there have been no applications over large spatial scales or long simulation periods.

An ongoing challenge is finding a balance between representing the complexity of the atmospheric chemistry, maintaining computational efficiency, and reproducing observed concentrations of pollutants. Performance objectives typically include predicting concentrations of ozone, components in particulate matter especially the acidic and organic components, and hazardous air pollutants as such as formaldehyde and acrolein. In addition, RAQMs have to accurately predict how concentrations respond to changing emission and climate scenarios.

The SAPRC series of mechanisms demonstrate one way to describe photochemistry needed to meet these objectives with a limited number of model species. Their approach is to lump organic chemicals by similarities in their reaction rates and products. The SAPRC07 mechanism (Carter, 2010a, b) updates the SAPRC-99 mechanism and has been peer reviewed and evaluated. (Azzi, 2010; Derwent, 2010; http://www.arb.ca.gov/research/reactivity/rsac.htm)

In this study, we use the Community Multiscale Air Quality (CMAQ) model (Byun and Schere, 2006) to test the predictions and the behavior of the SAPRC07 mechanism. CMAQ is a 3-D air quality model that is widely used for regulatory and research applications (Lin et al., 2010, Yu et al., 2010 and Lee et al., 2007). The model is now being used to examine the effects from proposed emission controls on a multi-pollutant basis - the simultaneous effects on concentrations of ozone, fine particulate matter ($PM_{2.5}$), and hazardous air pollutants (HAPs) in one simulation. Previous evaluations of the CMAQ model have been performed for ozone (Yu et.al., 2010 and Appel et al., 2007) and $PM_{2.5}$ components (Appel et al., 2008 and Chen et al. 2008) using either the CB05 or SAPRC-99 mechanism.

A recent study describes an early implementation of gas-phase SAPRC07 over a domain covering the U.S. state of California for several days in May (Cai et al., 2011). It compared predictions against observation and investigated how predictions changed with reduction of nitric oxide (NO) and nitrogen dioxides (NO_2), collectively referred to as NO_x, emissions. The application described in this paper differs from that effort by implementing a version of SAPRC07 that adds species for HAPs, specific ozone precursors, and secondary aerosol production. The application also covers a larger domain and longer simulation periods. In addition, the application uses process analysis to diagnose differences in predictions against predictions from the SAPRC-99 mechanism and compares predictions with observations for gas and aerosol-phase species. Objectives of this paper are twofold: (1) to determine if using this extended version of SAPRC07 would improve our ability to accurately simulate multiple pollutants, (both ozone and $PM_{2.5}$), and (2) to provide information to support the use of SAPRC07 in the CMAQ model for regulatory and research purposes.

2. Methods

2.1 The Model and Simulations

For this study, we used CMAQ version 4.7.1 (Foley et al., 2009). The domain had 14 vertical layers and simulations were performed over two grids: one with a 36X36 km^2 horizontal resolution covering the continental U.S., and the other with a nested 12X12 km^2 horizontal grid resolution covering the Eastern U.S. (Figure 1). Boundary conditions for the continental CMAQ simulations were extracted from the GEOS-CHEM model (http://acmg.seas.harvard.edu/geos/index.html; Bey et al., 2001) and mapped to CMAQ species based on Byun and Moon (2010). Boundary conditions for the nested domain were provided by the continental simulations. The simulations were performed for two monthly periods covering January and July, 2002, excluding a 10-day spin up period. Meteorological inputs were obtained from the MM5 meteorological model (http://box.mmm.ucar.edu/mm5/) version 3.6.1.

2.2 Emissions

We extracted emissions for January and July from the 2002 National Emission Inventory (NEI) (http://www.epa.gov/ttn/chief/net/2002inventory.html). Emissions of lumped model

species were allocated according to speciation rules provided for each mechanism (http://www.cert.ucr.edu/~carter/emitdb/). Biogenic emissions were calculated with Biogenic Emissions Inventory System (BEIS) v3.12 (http://www.epa.gov/asmdnerl/biogen.html). Emissions were processed with SMOKE v.2.0 (http://www.smoke-model.org). Emissions of the HAP species were extracted directly from the NEI, while other VOCs were derived based on speciation of the VOC profiles (Simon et al., 2010).

2.3 The Chemical Mechanism

The original SAPRC07 mechanism has been described in detail elsewhere (Carter, 2010a, b). The most significant changes include an update to the method for representing aromatics, a 19% increase in the reaction rate of hydroxyl radical (OH) with NO_2, a more detailed representation of products formed at low NOx conditions, and increased photolysis of formaldehyde (HCHO). In this study, we used the SAPRC07T version, which differs from the standard SAPRC07 mechanism because the mechanism includes additional species that permit more accurate simulation of reactive organic compounds (such as propene, ethanol, 1,2,4-trimethylbenzene) and HAPs (such as acrolein, 1,3-butadiene, toluene, isomers of xylene). The former species include compounds that are emitted in large quantities or suspected to form Secondary Organic Aerosols (SOA) either by gas phase or cloud droplet chemistry (glycoaldehyde, sesquiterpenes, and alpha-pinene). Because these compounds can comprise large percentages of the standard lumped SAPRC07 model species, reaction rates and coefficients of model species have been modified accordingly. The mechanism is described in the Supplementary Material Tables S-1 thru S-5. The version of SAPRC07T implemented in the CMAQ model is SAPRC07TB (http://www.cert.ucr.edu/~carter/SAPRC/files/MECH/SAPRC07T/S07TB.MEC), one of two variants available. The other is SAPRC07TC. The variants have the same species and give the same predictions but differ in the numerical expressions of reaction rate constants. The CMAQ implementation of SAPRC07T includes the photolysis cross sections and quantum yields evaluated in the SAPRC07 mechanism, but we have introduced temperature and pressure dependencies into photolysis reactions based on expert recommendations (Sander et al., 2006).

While the SAPRC07 and SAPRC07T mechanisms were not developed to predict production rates of secondary aerosols, both mechanisms predict concentrations of compounds

that produce species found in particle matter such as sulfate, nitrate, and organic material. We have extended the SAPRC07T mechanism to be compatible with the AERO5 aerosol module in CMAQ (Foley et al., 2009) to calculate aerosol concentrations by adding reaction products that enable secondary aerosol formation. Nitrate and sulfate concentrations in particulate matter are calculated by using ISORROPIA, an equilibrium thermodynamics module that partitions inorganic compounds between gas and particle phases (Nenes et al., 1999). The AERO5 module includes two heterogeneous reactions that occur on the water in aerosols. One consumes gaseous dinitrogen pentoxide (N_2O_5) to produce nitric acid (HNO_3). The other uses gaseous NO_2 to produce nitrous acid (HONO) and HNO_3 (Sarwar et al., 2008). Both reactions influence the aerosol nitrate. Concentrations of SOA in CMAQ AERO5 are mainly determined by homogeneous reactions between organic compounds with ozone, OH, NO_x and nitrate radicals. The products reversibly partition between gas and aerosol phases based on their sub-cooled liquid vapor pressures. A reaction within cloud droplets is a minor source of SOA by reactions between dissolved OH and Glyoxal or Methyl Glyoxal (Carlton et. al., 2010). Organic particulate matter from emissions is assumed nonvolatile. Several emitted components of inorganic particulate matter such as elemental carbon are assumed chemically inert. In essence, the mechanism representing particulate matter is the same between SAPRC99 and SAPRC07T implementations in the CMAQ model, but the concentrations of PM components can differ because of differences in the predictions of the gas phase precursors.

2.4 Method of Analysis

To better interpret predictions of SAPRC07T and how they have changed from SAPRC-99, we show predictions of regional concentrations and compare them to results from SAPRC-99. Our focus includes both differences in the average and maximum concentrations over and within the two simulation periods. To identify the reactions explaining why predictions differ between the mechanisms, we have applied Integrated Reaction Rate (IRR) and process analysis available in the CMAQ model (Gipson, 1999; Jeffries and Tonnesen, 1994). We present this information for three days at several locations with the model domain (Figure 1).

To determine whether the SAPRC07T mechanism improves performance in reproducing observations, we compare predictions from both mechanisms with observations from EPA's AQS database (http://www.epa.gov/air/data/aqsdb.html). For ozone, our comparison uses

maximums of the 8-hour averages. For components measured in $PM_{2.5}$, we compare 24 hour averages. Results are aggregated into geographical regions for both ozone and aerosol comparisons by using Principal Component Analysis (PCA) (Appel et al., 2008), as shown in Supplementary Figure S-1. The regional and IRR analysis allows interpreting whether differences between predictions and observations come from problems in simulation inputs such as emission and meteorological data or shortcomings in the photochemical mechanism.

3. Results and Discussion

3.1 SAPRC07T and SAPRC-99 comparisons for Ozone

Figure 2 shows monthly averages and maximums in the 8-hour averages in predicted ozone averaged for January and July 2002. Monthly averages for January are half as much as July, because higher temperatures, actinic fluxes and biogenic emissions increase photochemical production of ozone during the summer months. Maximums in the 8-hour average (bottom, Figure 2), relevant for regulatory policy, can be double the monthly averages.

Ozone predictions from SAPRC07T generally have lower concentrations than SAPRC-99. Differences averaged over the domain are about 0.2 ppb for January and 1 ppb for July. Many areas show maximum differences around 8-20 ppb lower for SAPRC07T, mostly in areas with high NO_x concentrations, such as along the Ohio River Valley (Figure 2-f). The largest differences occur mainly in urban areas where NO_x concentrations or emissions are high relative to volatile organic hydrocarbons (VOCs) (Supplementary Material Figure S-2, for the Great Lakes PCA). Some locations do show greater ozone predictions from SAPRC07T than from SAPRC-99 but the amounts are less than 5 ppb. The locations occur at rural and less developed areas that have the opposite trends in VOCs to NO_x ratios. For example, Figure 3 shows predictions from two grid cells. At "CHI" located in Chicago, SAPRC-99 predicts greater concentrations of ozone than SAPRC07T. The location labeled "ALA" shows the opposite relation between SAPRC-99 and SAPRC07T. This location has lower NO_x and higher biogenic VOCs.

IRR analysis enables us to identify which reactions cause the above differences. In SAPRC07T, NO_2 photolysis increases by 8% and is the main route for ground state oxygen atom ($O(^3P)$) production leading to ozone formation. The higher photolysis rate causes larger ozone

formation in SAPRC07T than SAPRC-99, especially in high NO_x areas (Figure 4a). Although SAPRC07T forms more ozone, it destroys more ozone in urban areas (Figure 4b) because the titration of ozone by NO is 8% higher in SAPRC07T and is the largest contributor to ozone destruction in these areas (Figure 4c). Even though ozone titration produces NO_2 that can recycle the destroyed ozone, recycling does not have perfect efficiency because other reactions destroy NO_2, such as the OH + NO_2 termination reaction. In some rural areas with lower NO_x concentrations, higher photolysis of NO_2 produces greater ozone concentrations from SAPRC07T because low NO makes titration a less important sink for ozone while OH concentrations are generally lower outside urban areas, i.e., less NO_2 termination.

A dominating factor in the above explanation is that SAPRC07T uses a rate constant for NO_2 + OH reaction that is 19% higher than SAPRC-99 (Carter, 2010a). Despite the higher rate constant, SAPRC07T can predict less HNO_3 production in areas where the OH concentrations are higher in SAPRC-99 (Figure 5d) especially during the afternoon when the OH differences between the two mechanisms are magnified. The differences decrease in the late afternoon as the solar forcing decreases. Other pathways producing HNO_3 also vary over the day and differ between mechanisms. On average, the homogeneous reactions between N_2O_5 and water contribute about 2-3% and > 1% of the total HNO_3 in SAPRC-99 and SAPRC07T, respectively. Note that the above HNO_3 differences are small so that SAPRC07T and SAPRC-99 produce similar concentrations.

While on average ozone predictions do not change substantially with using SAPRC07T, it predicts larger differences in several species that affect ozone chemistry and atmospheric reactivity. Figure 5 shows differences in two radicals, OH and hydroperoxyl radical (HO_2), and two compounds, HCHO and HNO_3 which affect radical cycles. Differences in peroxyacetyl nitrate (PAN) concentrations are shown in Supplementary Figure S-3. In general, SAPRC07T predicts lower OH concentrations and predicts higher HO_2, except in areas with large NO_x emissions. The latter result contradicts Cai *et al.* (2011) and may occur from differences in biogenic emission between the separate model domains. Updates in SAPRC07T that explain the difference are rate constants controlling the OH cycling. For example, OH production is reduced because updates lower the rate constant for the reaction of electronically excited oxygen atom ($O(^1D)$) with water. The reaction accounts for 10-25% and 30-45% of OH production over urban areas and rural areas, respectively. SAPRC07T also creates less OH from HO_2 (Figure 6a and

6d), despite that the HO_2+NO reaction has a slightly higher rate constant in SAPRC07T. The increased rate does produce slightly greater HNO_3 concentrations from SAPRC07T

Formaldehyde has lower concentrations with SAPRC07T for two reasons. First, the HCHO photolysis rate forming radicals increases 19% (Sander et al., 2006). Second, SAPRC07T splits HCHO production into direct and indirect processes unlike SAPRC-99. HCHO is directly formed in SAPRC07T as a reaction product and indirectly through operators produced by reactions. The operator has a HCHO yield equal to 100% when it reacts with NO, NO_3, acetyl peroxy and peroxyacyl radicals. Reactions with alkoxy radicals have a yield equal to 50%. No HCHO is formed when the operator reacts with HO_2 radicals. The net effect decreases HCHO production, especially in low-NOx areas. Because HCHO and other carbonyl compounds are a source of HO_2 radical, this reduces HO_2 production via organic compounds. Figure 6c illustrates how the lower formaldehyde concentrations affect the sources of HO_2. Luecken et al. (2011) evaluated of the HCHO predictions from SAPRC07T. Predictions generally underestimated observations especially at the higher range of concentrations. Possible causes were errors in observational techniques that overestimate the actual concentration and the mismatch that exists when comparing observations at an exact location to grid cell averages predicted by a model. Predictions cannot include local effects on observations such as adjacent emission sources and subscale meteorology.

3.2 Comparison with Ozone Observations.

Predictions from SAPRC-99 and SAPRC07T have a similar agreement to observations of ozone (Table 1) for several statistical metrics. The metrics consider the daily maximums of the 8-hour averages measured at more than 700 sites throughout the domain. Normalized metrics are approximately within 20% for both months. January metrics generally show better agreement. Across the domain, SAPRC07T performs slightly better than SAPRC-99 (Figure 7, right), but the largest differences occur during July and are within two ppb for the period. They do not appear significant considering uncertainties in simulation inputs and each mechanism parameters. During July, the ozone bias changes with relative magnitude of ozone concentration. Model predictions tend to under estimate the high range of 8-hour maximums while overestimating the lowest observed concentrations. The bias correlates with the isoprene concentrations: a positive ozone bias occurs at sites where isoprene is predicted to be the highest

(Figure S-4). At low isoprene, biases are more symmetrically positive and negative, but dominantly positive at the highest isoprene sites.

To interpret the results, we aggregated results by geographical region and compared one hour averages of model predictions and observations. With these aggregations, the performance varies across the domain and with time of day. The bias appears the worse in the Southern and Southern Atlantic regions of the domain (Figure 8). The region is well known for high emissions of isoprene and other biogenic compounds. Previous evaluations have noted the above behavior in model bias (Appel et al., 2007). When comparing predictions to observations based on time of day, the model performs worse in the morning and evening hours when compared to daytime conditions. Supplementary Figure S-5 presents statistics for the four PCA regions when computed as a function of morning/evening (4:00 PM to 7:00 AM) versus daytime (7:00 AM through 4:00 PM). Ozone is predicted better in the afternoon but over predicted in the morning. The problem is more obvious in the southern U.S.

The causes are difficult to untangle because predictions involve several processes: emissions, meteorology, chemistry, deposition, boundary conditions, etc. Dynamic evaluation studies indicate errors in the emissions inventory or transport above the nighttime boundary layer such as the nocturnal jet and boundary conditions for the upper troposphere (Godowitch et al, 2010). Emission inventory errors are frequently suspected in ozone simulations. Their errors remain difficult to quantify but often occur through the temporal and spatial allocation of emissions especially in urban areas. In particular, NOx emissions suffer errors because their anthropogenic sources are poorly resolved by simulation's grid cell resolution. On the other hand, the relation between model bias and isoprene predictions suggest errors in biogenic emissions and models for biogenic emissions vary in predicted isoprene and other volatile organic compounds by a factor of two (Luecken et al., 2011). Errors in transport and boundary conditions will also cause the simulations to inaccurately move ozone and its precursors between grid cells which will affect where and the degree to which ozone production and radical cycles are initiated and simulated in a given grid cell. Poor performance at higher isoprene concentrations and the southern locations also point to potential errors in meteorological inputs, including errors in the morning boundary layer height, nighttime transport and deposition. They can lead to the positive biases during morning hours that persist into latter into day, especially at sites with the lowest averages (Godowitch et al., 2010).

We also suspect errors in the photochemical mechanism. Comparisons with smog chamber show that the original SAPRC07 gives satisfactory performance for a single compound at simulations representing urban conditions but the simulations did not robustly cover conditions at low VOC/NOx ratios (Carter, 2008). The same ratios exist at locations in our simulations where SAPRC07T and SAPRC-99 prediction show the largest differences. We conclude that predictions are most uncertain in these areas. Reaction rate constants and photolysis rates contribute to these uncertainties. Cohan et al. (2010) studied rate constants that introduce the most uncertainties into model predictions at such VOC/ NO_x ratios. They identified the rate constant for the NO_2 + OH reaction as the largest source. Their conclusion is relevant to differences between our predictions and IRR analyses from SAPRC-99 and SAPRC07T. The reaction's rate constant uses a Lindemann-Hinshelwood type of expression and remains uncertain because several of reactants and products are difficult to measure accurately. Mollner et al. (2010) illustrate this point by measuring branching ratios that differed from previous IUPAC and NASA/JPL recommendations (Atkinson et al., 2006; Sander et al., 2006). Mollner et al. also determined that their measurements infer increases in ozone up to 10% over Southern California, a low VOC/ NO_x area. We have performed sensitivity studies using this lower rate constant and it lowers the differences between SAPRC07T and SAPRC-99 (Supplementary Figure S-6).

Our IRR analyses also indicated that several photolysis rates and reactions dependent on photolysis products cause large differences between the two mechanisms. The findings are important for low VOC/NO_x areas because they affect ozone and OH production rates. Cohan et al. (2010) also identified that the photolysis rate of NO_2 introduces large uncertainties in ozone predictions because the reaction has a key role in ozone production and has photolysis parameters that are less well defined across wavelength. Their conclusion is supported by Hanna et al. (2001) and is illustrated by comparing NASA/JPL reviews of photochemical data (Sander et al. 2006 and Sander et al. 2002). Cohan et al. did not address actinic fluxes that are used to calculate photolysis rates. In our simulations, photolysis rates were calculated off-line and did not vary as a function of surface albedo based on land use. Over a global domain, Laepple *et al*. (2005) found regression slopes for the NOx and OH to changes in surface albedo equal to 20.02% and 170.1%, respectively. Effects on ozone are difficult to estimate on regional and urban scales because both ozone production and loss showed large changes and because of the

domain size and grid cell sizes used in their simulations. Our tests that assessed ozone sensitivity to albedo found summertime changes in predictions between 5 to 15% and -3% to -10% over low and high VOC/NOx areas, respectively.

3.3 $PM_{2.5}$ and aerosol components

The aerosol sulfate and nitrate predictions from SAPRC07T are shown in Figure 9. Aerosol concentrations predicted by the CMAQ model can be divided into two components dependent on gas phase chemistry. One, the inorganic or aqueous component, includes sulfate and nitrate. Sulfate production relies on OH and hydrogen peroxide (H_2O_2) concentrations through homogeneous and in-cloud (i.e., aqueous phase) pathways, respectively. Simulations that used the SAPRC07T mechanism predict smaller sulfate concentrations because of its lower OH and H_2O_2 concentrations with its lower OH concentrations as the prevalent cause because the sulfate differences strongly correspond to the OH differences between the two mechanisms. Aerosol nitrate using SAPRC07T is slightly smaller than using SAPRC-99 (Supplementary Material Figure S-8), where the former produces lower HNO_3 concentrations (Figure 5). SAPRC07T does produce greater concentrations of aerosol nitrate because its lower sulfate concentrations favor HNO_3 absorption into the aqueous aerosol component based on the thermodynamic equilibrium model, ISOROPPIA. However, differences in nitrate can also occur because small sulfate differences can produce discontinuous caused by numerical algorithms within ISOROPPIA. The other component dependent on gas phase chemistry is the Secondary Organic Aerosol (SOA) component. Production of SOA relies on O_3, HOx and NOx concentrations (Supplementary Material Table-S1). SAPRC07T generally predicts lower concentrations that correspond to its lower predicted NOx concentrations in the southeastern states.

Although SAPRC07T predicts lower values of the individual aerosol species and total $PM_{2.5}$, we find similar agreement between predictions from both SAPRC07T and SAPRC99 with observations (Figure 10). The values are also consistent with previous reported ranges of predictions from the CMAQ model (Appel et al., 2008). Comparison results from the mechanism vary slightly between geographical regions (Figure 11), arising from different production rates of

inorganic and organic aerosol mass that depend on gas phase concentrations of oxidants and radicals. The small differences between the two mechanisms indicate that physics and parameterizations within the aerosol module determine aerosol concentrations more than the gas phase chemistry.

4. Summary

Numerous changes in the reaction rates, secondary reactions, products, and organic speciation were made in order to update SAPRC-99 and produce SAPRC07. The SAPRC07T mechanism implemented into the CMAQ model extends SAPRC07 to better represent HAPs, secondary aerosol precursors and VOCs such as propene and ethanol. SAPRC07T explicitly predicts atmospheric species needed to assess air quality, ecological damage and human exposure to criteria and hazardous pollutants. The mechanism then provides a tool for developing multi-pollutant control strategies that not only focus on ozone and $PM_{2.5}$, but include HAPs, greenhouse gases, visibility, etc.

Overall, predictions of ozone and $PM_{2.5}$ did not significantly change when the CMAQ model used the SAPRC07T mechanism instead of SAPRC-99, despite a large number of changes made to create the SAPRC07T mechanism. Differences in ozone predictions mostly arise from changes to the inorganic reactions, such as photolysis of NO_2 and destruction of ozone by NO. Changes or updates in the NO_2 + OH reaction are moderated by lower OH production via the reaction of $O(^1D)$ with water. These consequences demonstrate that updates to inorganic chemistry can overwhelm efforts to improve the representation of organic chemistry, in terms of influence on ozone predictions. If ozone predictions remain a major focus in developing RAQMs, emphases should be placed on reducing uncertainties in inorganic reactions rate constants and their parameters such as actinic fluxes.

Our analysis indicates that the model over estimates ozone concentrations during the early morning hours in the summer. Comparisons to observations show that the problem is

especially large over south eastern regions in the United States. This problem occurred for both mechanisms used.

Model performance studies often focus on reproducing ozone maximums, not the hourly concentrations and their diurnal variations. SAPRC07T better matches the maximums than the time series of hourly concentrations. However, the latter performance issue is becoming increasingly important when implementing secondary standards to protect vegetation, to assess long-range transport and to address potentially lower ozone standards. We then have to determine what factors deteriorate model performance at all hours of the day. For example, nighttime chemistry has received little attention relative to daytime photochemistry so can missing chemical or physical processes cause over predicted concentrations during nighttime to affect early morning hours? As stated earlier, meteorological parameters such as nighttime transport, boundary layer heights, and mixing have potential errors and significant impacts. Also, emission inventories remain an important error source, specifically NO_x and isoprene emissions. However, emission errors are unlikely to explain over-predictions because potential corrections in isoprene, such as using an alternative model for biogenic emissions, would probably produce even higher ozone predictions during the morning hours.

Progress has been made at improving chemical mechanisms but many aspects of ozone production and loss remain unidentified or uncertain. Are there reactions completely missing that would improve model predictions such as heterogeneous reactions? Such improvements may have a role but the predicted concentrations result from the interplay between atmospheric chemistry, physics, meteorology and emission processes, which will be difficult to define by only improving the chemical mechanisms. For example, the SAPRC07T mechanism incorporated changes to several key inorganic reactions but the changes produced small effects on overall ozone predictions and did not remove previously documented errors regarding comparison to observations. We conclude that both chemical mechanisms and RAQM inputs need greater improvements to better predict ozone during all hours of the day.

Given the uncertainties in the emissions and meteorological inputs, a fair question is what is gained by improving chemical mechanisms in RAQMs until the inputs improve above a defined level of confidence? For several reasons, chemical mechanisms still need improvements

in their representation of the production and loss of atmospheric compounds. Identifying errors in the emissions and meteorology may never end because the emissions sources continually change while chaotic and evolving factors drive meteorology. Improvements regarding their effects on air quality often rely on comparing observations and RAQM predictions. The effort assumes that RAQMs accurately represent the transport and fate of the emitted compounds. Chemical mechanisms play a key role in the simulated fate of most atmospheric pollutants so known errors within mechanisms must be minimized. Furthermore, RAQMs and their chemical mechanisms serve as a development base to address new scientific and environmental issues such as secondary particulate matter and toxic compounds. These efforts should use bases that incorporate a sound understanding of atmospheric chemical and physical processes. Finally, researchers and air quality managers currently use RAQMs to diagnosis air quality observations and to create plans for improving air quality. When chemical mechanisms do not incorporate the best data and theories within practicality, the diagnosis will contain errors and the plans may have unexpected consequences. Although research and development efforts may never remove all errors or shortcomings in chemical mechanisms, better mechanisms should continue to be developed, evaluated and implemented. These efforts should continue even when the current RAQMs satisfactorily reproduce observations, to ensure that the model's results are correct for the right reasons and that our understanding is not flawed, or based on compensating errors. Research and development of RAQMs need to consider new experimental measurements, chemical theories and computational techniques to improve how they represent atmospheric chemistry, so they better support more efficient and effective pollution control strategies.

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Table 1: Performance measures for predicted 8 hour daily maximum in ozone from of SAPRC07 and SAPRC-99 Ozone (ppb) during January and July, 2002. The central columns for July are based on the same observational sites available during January.

	January		July with January Sites		July at All Available Sites	
	SAPRC07	SAPRC99	SAPRC07	SAPRC99	SAPRC07	SAPRC99
Correlation coefficient	0.7	0.7	0.8	0.8	0.8	0.8
Root Mean Square Error	7.59	7.46	12.9	13.7	12.4	13.6
Mean bias	-1.37	-1.11	5.9	7.6	5.2	7.1
Normalized mean bias	-5.1%	-4.1%	11.7%	15%	9.2%	12.6%
Mean error	5.86	5.77	10.3	11.0	9.73	10.6
Normalized mean error	21.8%	21.5%	20.5%	21.8%	17.2%	18.8%

FIGURE CAPTIONS:

Figure 1. Simulations used two domains: a parent 36X36 km^2 and nested 12X12 km^2 domains. The labeled locations are used in the detailed process analysis.

Figure 2. Ozone concentrations predicted by SAPRC07T are shown (a) averaged over January, (c) averaged over July, and (e) the maximums of the 8-hour averages during July. Subfigures (b), (d) and (f) show the differences between SAPRC07T and SAPRC-99 for the statistic on the left.

Figure 3. Ozone concentrations from each mechanism are given for two locations where the differences between mechanisms reverse in sign. At the Chicago (left), SAPRC-99 predicts higher ozone, while at the southern Alabama (right), SAPRC07T predicts higher ozone. The hourly values of ozone concentrations and differences are shown from July 15 to 17, 2002.

Figure 4. Ozone production and decay processes are displayed for six locations from July 15 to July 17: (a) total ozone production, (b) net ozone loss; (c) fraction of ozone loss due to titration; and (d) fraction of ozone loss due to photolysis. The solid bars indicate processes within SAPRC07T and hatched lines are the corresponding rates for SAPRC-99.

Figure 5. Differences between SAPRC-99 and SAPRC07T are displayed for (a) HCHO, (b) OH, (c) HO_2, and (d) HNO_3. For HCHO, differences are on the order of 15%. For HNO_3, they are less than 5%. Differences in OH and HO_2 can be up to -30% in high-NO_x areas.

Figure 6. At six locations, processes affecting OH production are given from July 15 through July 17: (a) net OH produced from HO_2; (b) total HNO3 produced through OH+NO_2 reactions; (c) production of new HO_2 from formaldehyde photolysis; and (d) resulting ratio of the OH to the HO2 concentrations.

Figure 7. The figure displays spatial distribution of the Normalized Mean Bias (NMB) displays for SAPRC07T in January (a) and in July (c). It also shows how the NMBs changes between predictions from SAPRC07T and SAPRC-99 for each month (b and d).

Figure 8: Average hourly concentrations of ozone for observations, SAPRC07T and SAPRC-99 for (a) Northeast, (b) Great Lakes, (c) South, and (d) Atlantic regions shown in Figure S-1. Subfigures on the left and right represent the January and July periods, respectively.

Figure 9. SAPRC07T predicted $PM_{2.5}$ sulfate (a and b) and nitrate (c and d), averaged over January (left) and July (right).

Figure 10. The scatter plots compare SAPRC07T predictions against observations of nitrate in $PM_{2.5}$ (a and b) and total $PM_{2.5}$ (c and d) during January (left) and July (right) periods.

Figure 11: The stacked bar plots compare predicted components of PM2.5 by SAPRC07T and SAPRC-99 against observations for the Figure S-1 regions: (a) Northeast, (b) Great Lakes, (c) South and (d) Atlantic regions. Subfigures display results for January and July on left and right, respectively

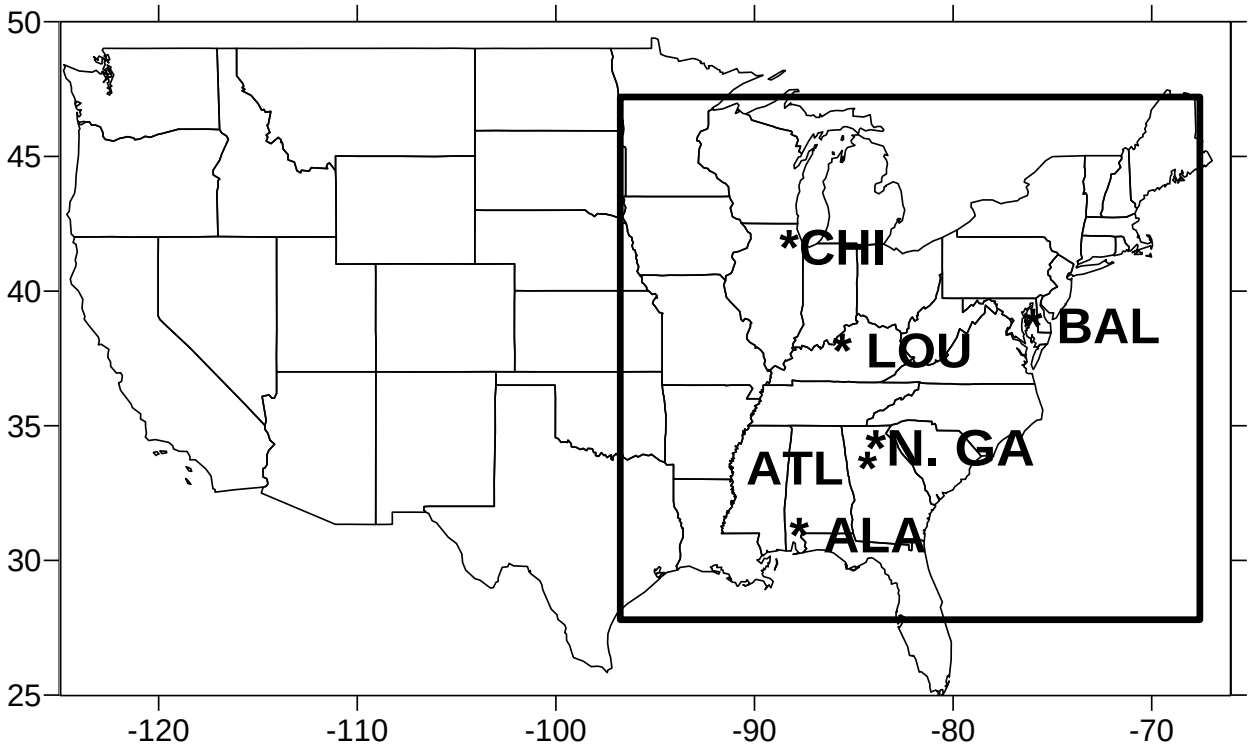

Figure 1.

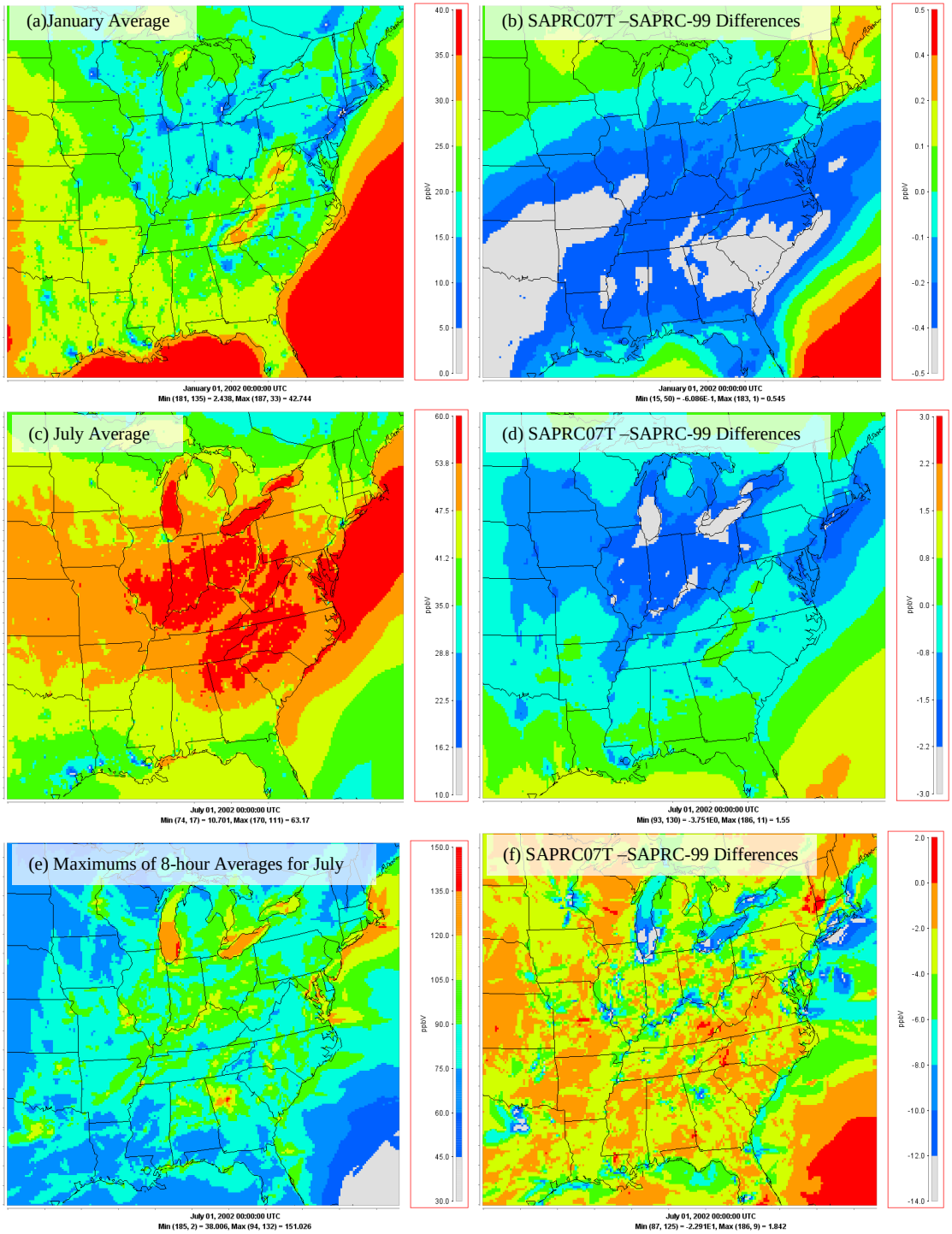
(a)January Average
(b) SAPRC07T –SAPRC-99 Differences
(c) July Average
(d) SAPRC07T –SAPRC-99 Differences
(e) Maximums of 8-hour Averages for July
(f) SAPRC07T –SAPRC-99 Differences
ppbV

Figure 2.

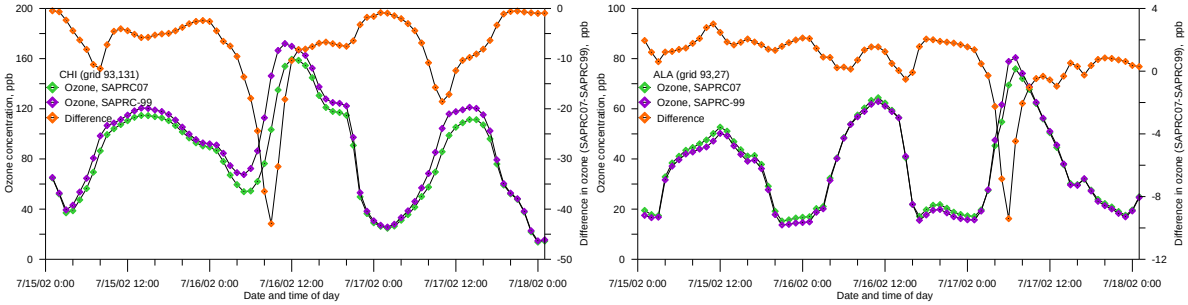
CHI (grid 93,131)
Ozone, SAPRC07
Ozone, SAPRC-99
Difference
Ozone concentration, ppb
Difference in ozone (SAPRC07-SAPRC99), ppb
Date and time of day
7/15/02 0:00
7/15/02 12:00
7/16/02 0:00
7/16/02 12:00
7/17/02 0:00
7/17/02 12:00
7/18/02 0:00
ALA (grid 93,27)
Ozone, SAPRC07
Ozone, SAPRC-99
Difference
Ozone concentration, ppb
Difference in ozone (SAPRC07-SAPRC99), ppb
Date and time of day

Figure 3.

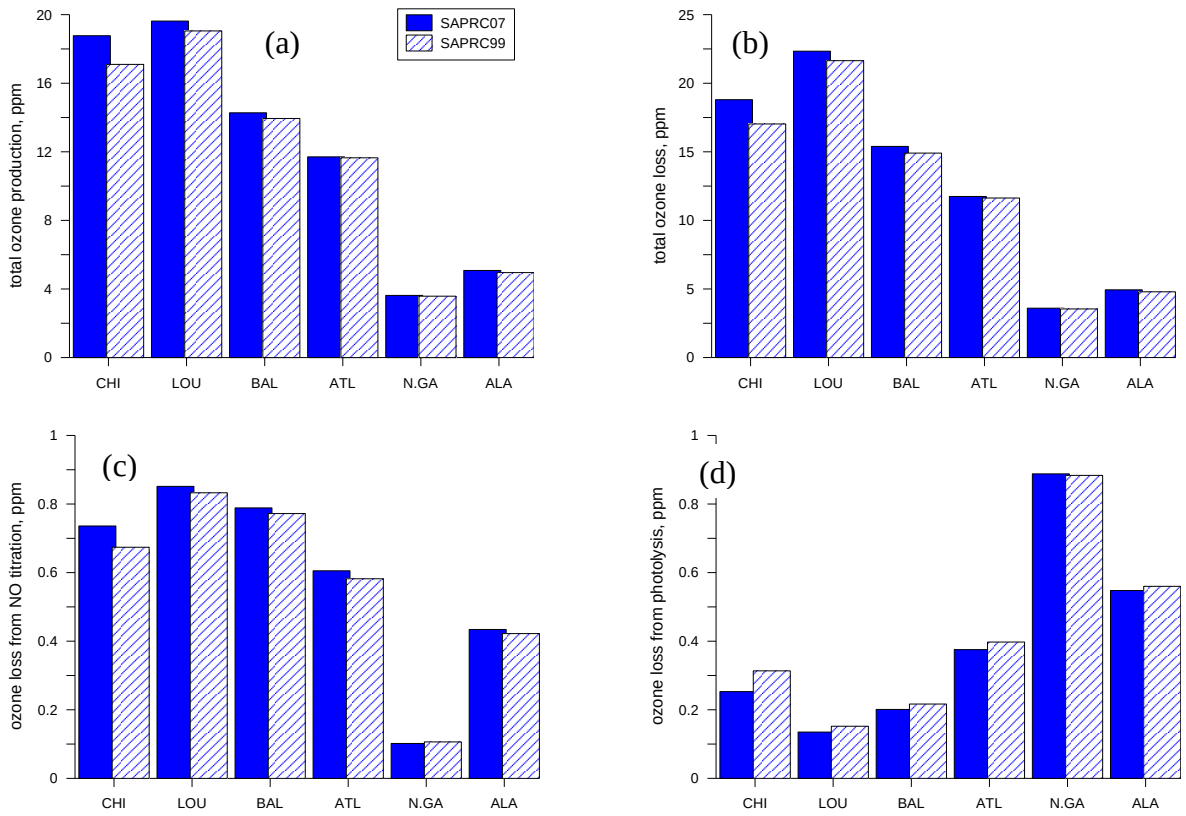
(a)
SAPRC07
SAPRC99
total ozone production, ppm
0
4
8
12
16
20
CHI
LOU
BAL
ATL
N.GA
ALA
(b)
total ozone loss, ppm
0
5
10
15
20
25
CHI
LOU
BAL
ATL
N.GA
ALA
(c)
ozone loss from NO titration, ppm
0
0.2
0.4
0.6
0.8
1
CHI
LOU
BAL
ATL
N.GA
ALA
(d)
ozone loss from photolysis, ppm
0
0.2
0.4
0.6
0.8
1
CHI
LOU
BAL
ATL
N.GA
ALA

Figure 4.

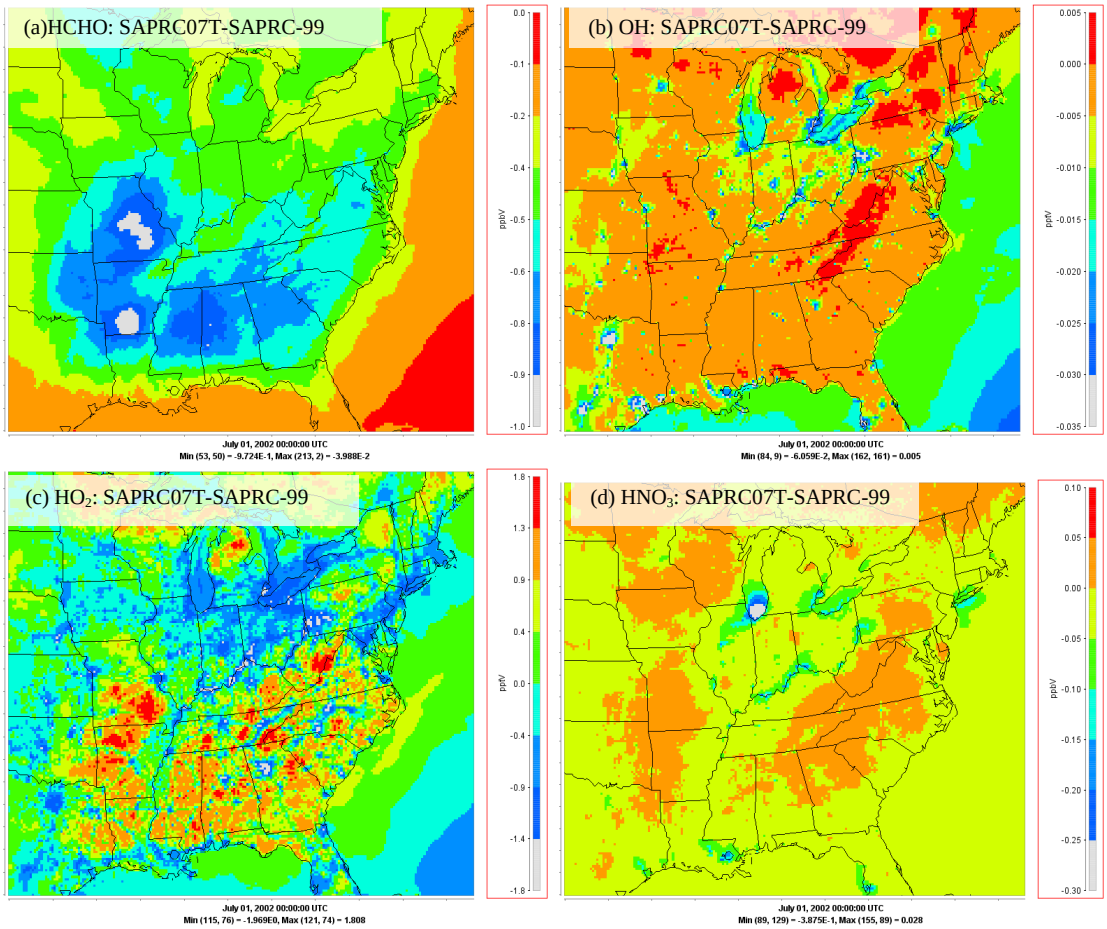
(a)HCHO: SAPRC07T-SAPRC-99
July 01, 2002 00:00:00 UTC
Min (53, 50) = -9.724E-1, Max (213, 2) = -3.988E-2
ppbV
(b) OH: SAPRC07T-SAPRC-99
July 01, 2002 00:00:00 UTC
Min (84, 9) = -6.059E-2, Max (162, 161) = 0.005
ppbV
(c) HO2: SAPRC07T-SAPRC-99
July 01, 2002 00:00:00 UTC
Min (115, 76) = -1.969E0, Max (121, 74) = 1.808
ppbV
(d) HNO3: SAPRC07T-SAPRC-99
July 01, 2002 00:00:00 UTC
Min (89, 129) = -3.875E-1, Max (155, 89) = 0.028
ppbV

Figure 5.

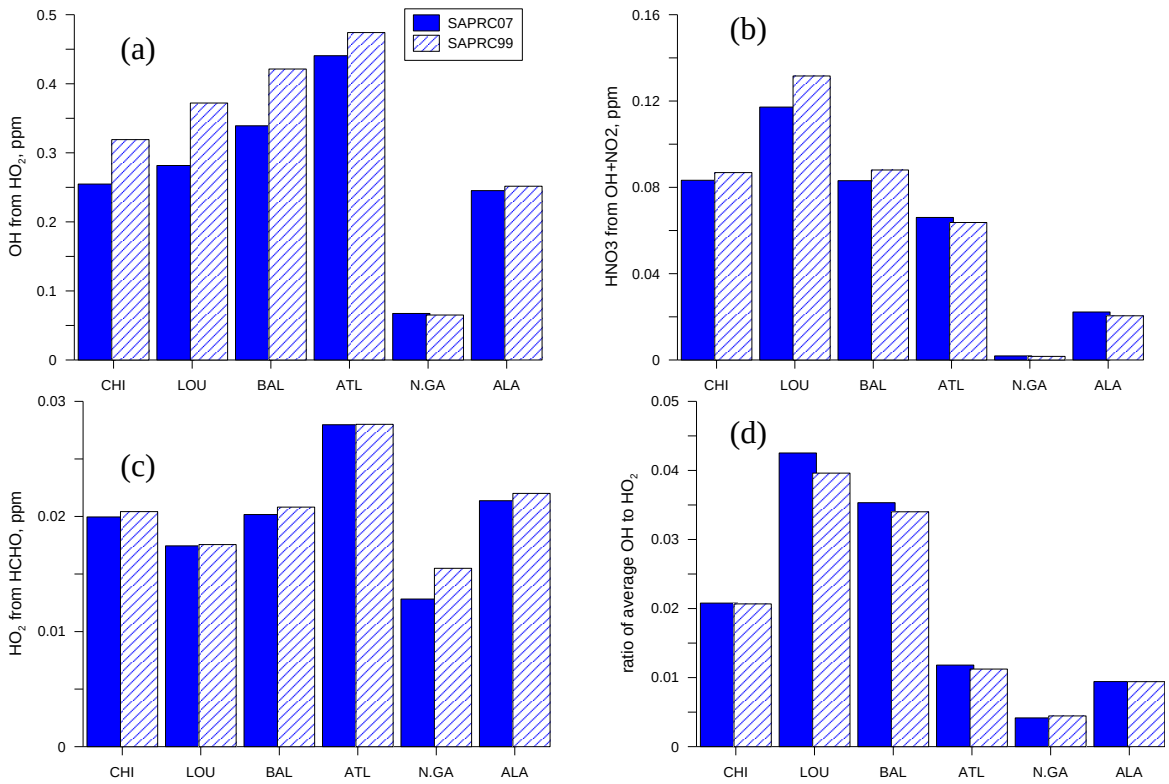
(a)
SAPRC07
SAPRC99
OH from HO2, ppm
0.5
0.4
0.3
0.2
0.1
0
CHI
LOU
BAL
ATL
N.GA
ALA
(b)
HNO3 from OH+NO2, ppm
0.16
0.12
0.08
0.04
0
(c)
HO2 from HCHO, ppm
0.03
0.02
0.01
(d)
ratio of average OH to HO2
0.05
0.04
0.03
0.02
0.01

Figure 6.

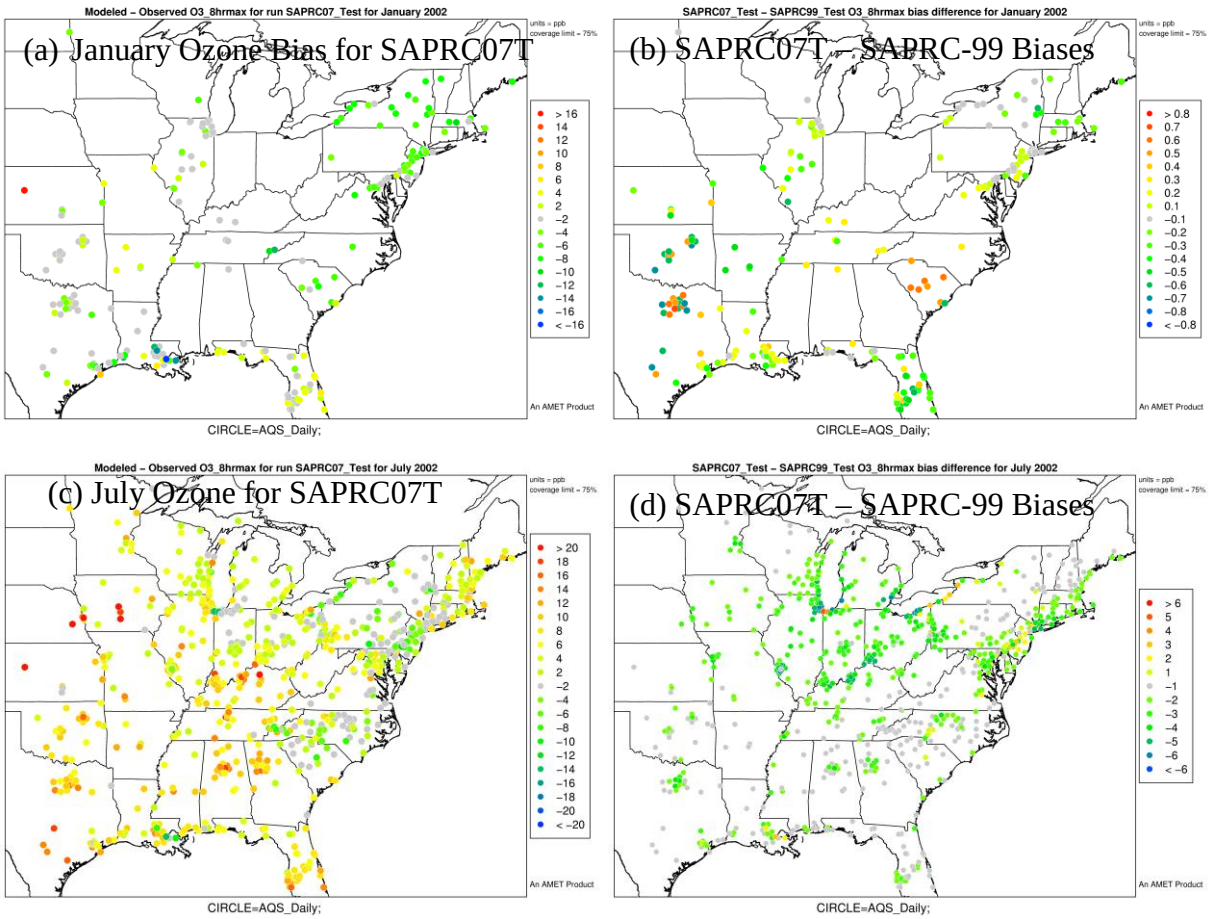
Modeled – Observed O3_8hrmax for run SAPRC07_Test for January 2002
(a) January Ozone Bias for SAPRC07T
SAPRC07_Test – SAPRC99_Test O3_8hrmax bias difference for January 2002
(b) SAPRC07T – SAPRC-99 Biases
Modeled – Observed O3_8hrmax for run SAPRC07_Test for July 2002
(c) July Ozone for SAPRC07T
SAPRC07_Test – SAPRC99_Test O3_8hrmax bias difference for July 2002
(d) SAPRC07T – SAPRC-99 Biases
CIRCLE=AQS_Daily;
An AMET Product

Figure 7.

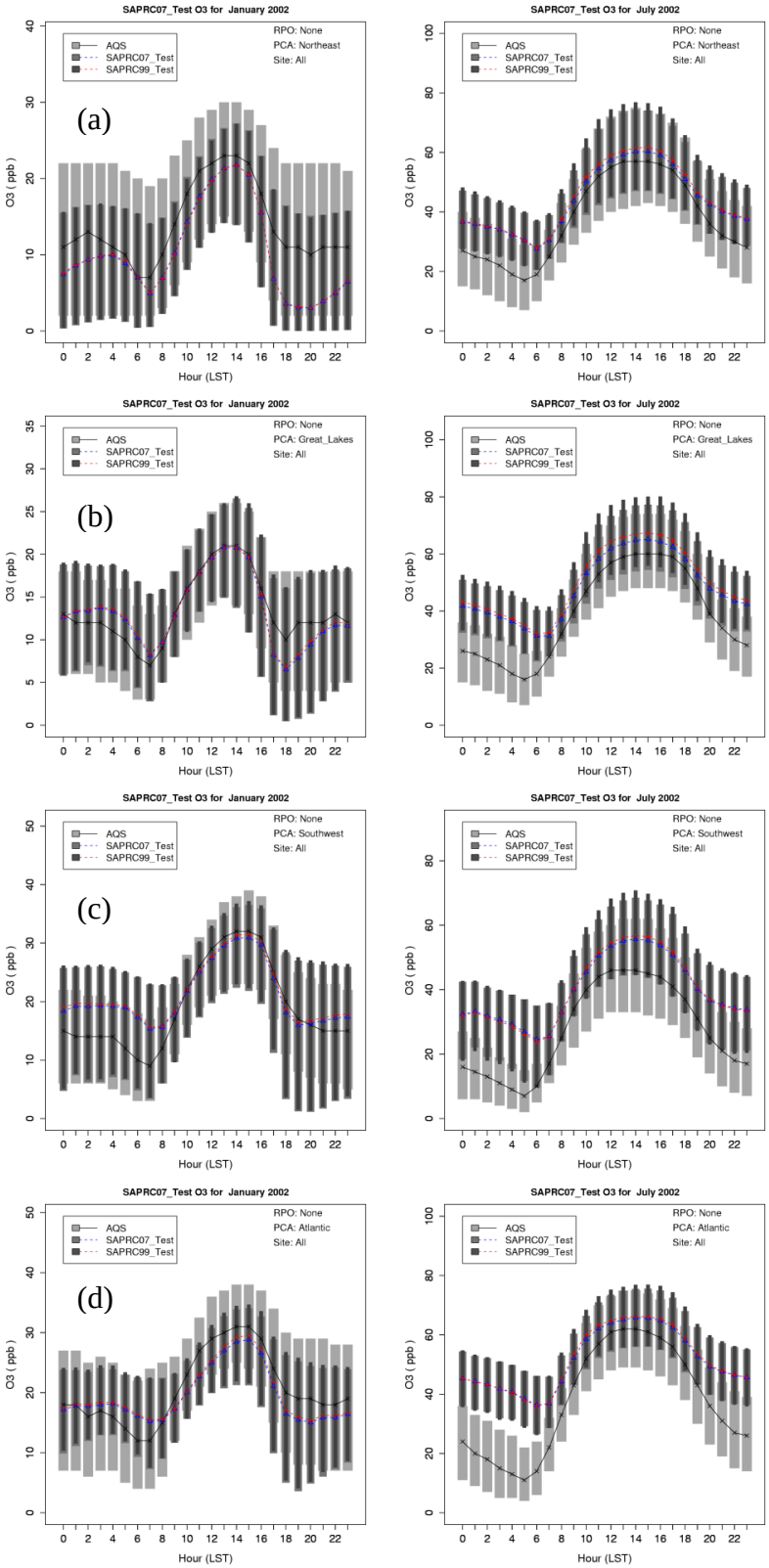
SAPRC07_Test O3 for January 2002
SAPRC07_Test O3 for July 2002
AQS
SAPRC07_Test
SAPRC99_Test
RPO: None
PCA: Northeast
Site: All
(a)
PCA: Great_Lakes
(b)
PCA: Southwest
(c)
PCA: Atlantic
(d)
O3 (ppb)
Hour (LST)

Figure 8.

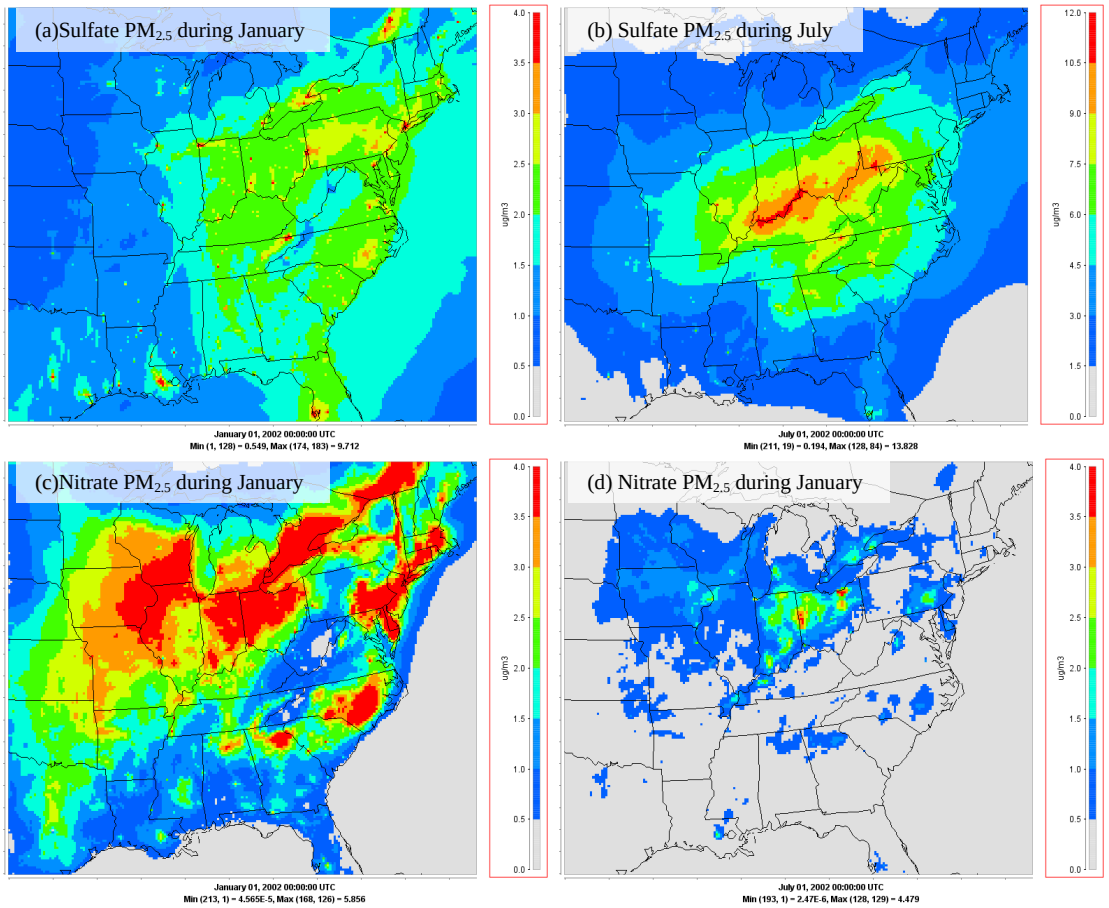
(a)Sulfate PM2.5 during January
(b) Sulfate PM2.5 during July
(c)Nitrate PM2.5 during January
(d) Nitrate PM2.5 during January
ug/m3
January 01, 2002 00:00:00 UTC
Min (1, 128) = 0.549, Max (174, 183) = 9.712
July 01, 2002 00:00:00 UTC
Min (211, 19) = 0.194, Max (128, 84) = 13.828
January 01, 2002 00:00:00 UTC
Min (213, 1) = 4.565E-5, Max (168, 126) = 5.856
July 01, 2002 00:00:00 UTC
Min (193, 1) = 2.47E-6, Max (128, 129) = 4.479

Figure 9.

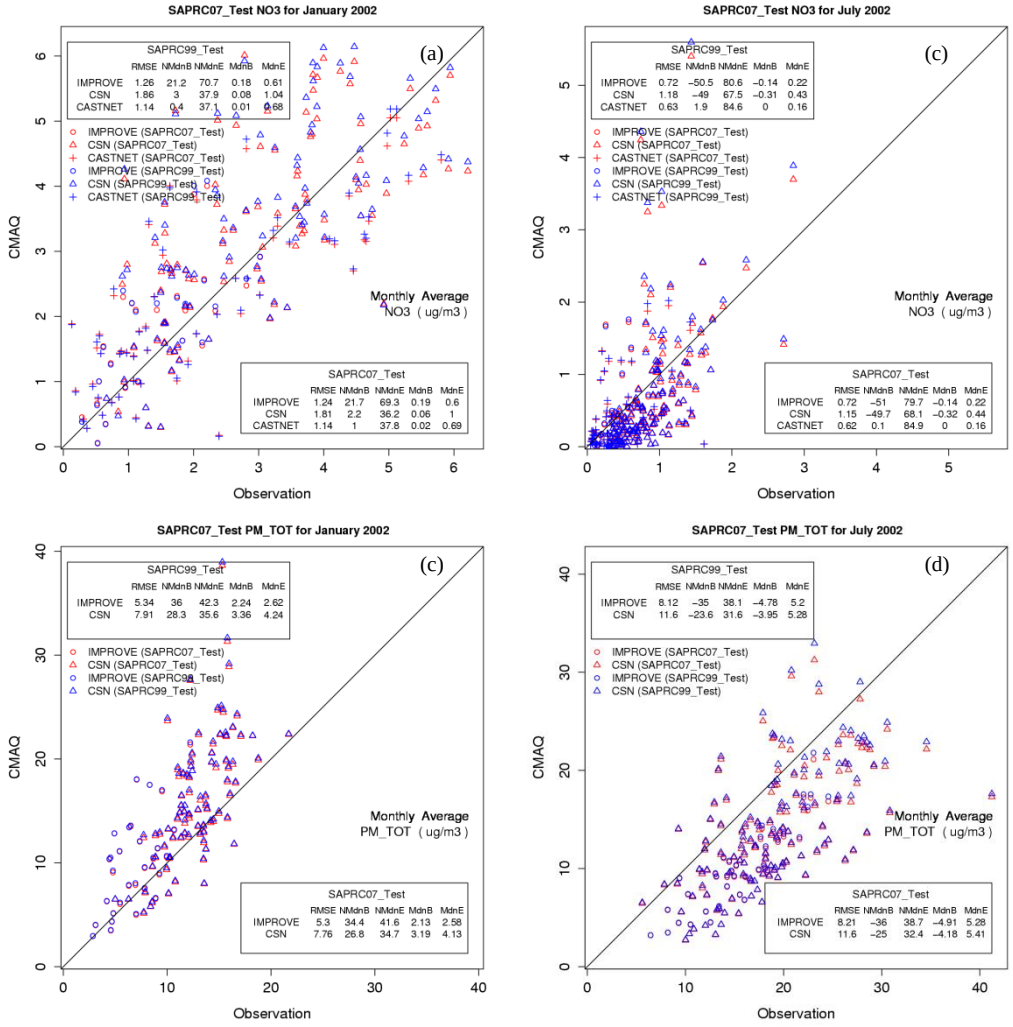
SAPRC07_Test NO3 for January 2002
(a)
SAPRC99_Test
RMSE NMdnB NMdnE MdnB MdnE
IMPROVE 1.26 21.2 70.7 0.18 0.61
CSN 1.86 3 37.9 0.08 1.04
CASTNET 1.14 0.4 37.1 0.01 0.68
IMPROVE (SAPRC07_Test)
CSN (SAPRC07_Test)
CASTNET (SAPRC07_Test)
IMPROVE (SAPRC99_Test)
CSN (SAPRC99_Test)
CASTNET (SAPRC99_Test)
Monthly Average
NO3 (ug/m3)
SAPRC07_Test
RMSE NMdnB NMdnE MdnB MdnE
IMPROVE 1.24 21.7 69.3 0.19 0.6
CSN 1.81 2.2 36.2 0.06 1
CASTNET 1.14 1 37.8 0.02 0.69
CMAQ
Observation
SAPRC07_Test NO3 for July 2002
(c)
SAPRC99_Test
RMSE NMdnB NMdnE MdnB MdnE
IMPROVE 0.72 −50.5 80.6 −0.14 0.22
CSN 1.18 −49 67.5 −0.31 0.43
CASTNET 0.63 1.9 84.6 0 0.16
IMPROVE (SAPRC07_Test)
CSN (SAPRC07_Test)
CASTNET (SAPRC07_Test)
IMPROVE (SAPRC99_Test)
CSN (SAPRC99_Test)
CASTNET (SAPRC99_Test)
Monthly Average
NO3 (ug/m3)
SAPRC07_Test
RMSE NMdnB NMdnE MdnB MdnE
IMPROVE 0.72 −51 79.7 −0.14 0.22
CSN 1.15 −49.7 68.1 −0.32 0.44
CASTNET 0.62 0.1 84.9 0 0.16
CMAQ
Observation
SAPRC07_Test PM_TOT for January 2002
(c)
SAPRC99_Test
RMSE NMdnB NMdnE MdnB MdnE
IMPROVE 5.34 36 42.3 2.24 2.62
CSN 7.91 28.3 35.6 3.36 4.24
IMPROVE (SAPRC07_Test)
CSN (SAPRC07_Test)
IMPROVE (SAPRC99_Test)
CSN (SAPRC99_Test)
Monthly Average
PM_TOT (ug/m3)
SAPRC07_Test
RMSE NMdnB NMdnE MdnB MdnE
IMPROVE 5.3 34.4 41.6 2.13 2.58
CSN 7.76 26.8 34.7 3.19 4.13
CMAQ
Observation
SAPRC07_Test PM_TOT for July 2002
(d)
SAPRC99_Test
RMSE NMdnB NMdnE MdnB MdnE
IMPROVE 8.12 −35 38.1 −4.78 5.2
CSN 11.6 −23.6 31.6 −3.95 5.28
IMPROVE (SAPRC07_Test)
CSN (SAPRC07_Test)
IMPROVE (SAPRC99_Test)
CSN (SAPRC99_Test)
Monthly Average
PM_TOT (ug/m3)
SAPRC07_Test
RMSE NMdnB NMdnE MdnB MdnE
IMPROVE 8.21 −36 38.7 −4.91 5.28
CSN 11.6 −25 32.4 −4.18 5.41
CMAQ
Observation

Figure 10.

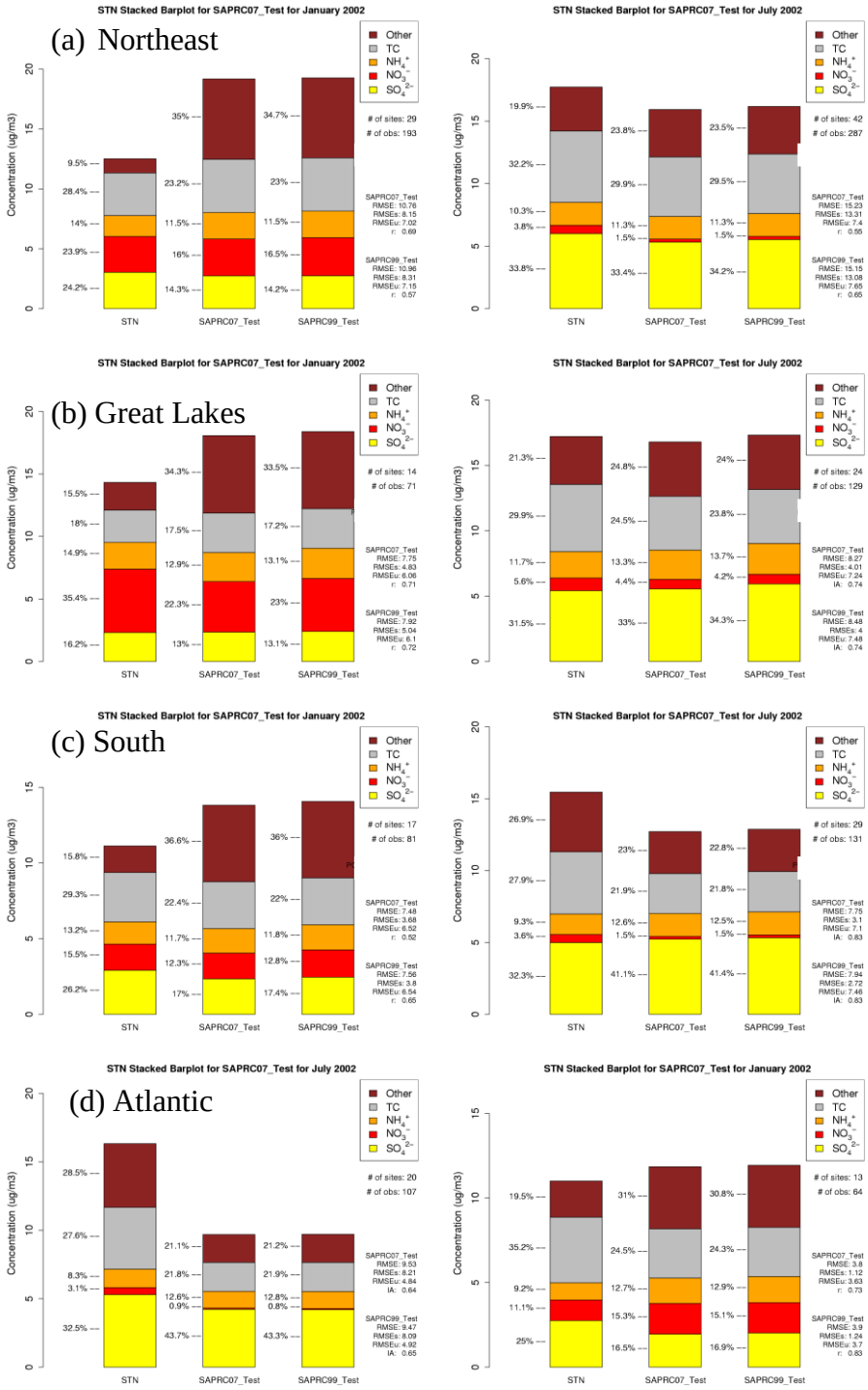
(a) Northeast
(b) Great Lakes
(c) South
(d) Atlantic
STN Stacked Barplot for SAPRC07_Test for January 2002
STN Stacked Barplot for SAPRC07_Test for July 2002
Other
TC
NH4+
NO3-
SO4 2-
Concentration (ug/m3)
STN
SAPRC07_Test
SAPRC99_Test

Figure 11.

1 Supplementary Material

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{1 }	NO2	--hv->	NO + O3P	NO2_06	See Table S-4
{2 }	O3P + O2 +M	--->	O3	k< 2> = 5.680E-34 * (T/300)**(-2.60)	
{3 }	O3P + O3	--->		k< 3> = 8.000E-12 * exp(-2060.0/T)	
{4 }	O3P + NO	--->	NO2	k< 4> is a falloff expression using: ko = 9.000E-32 * (T/300)**(-1.50) kinf = 3.000E-11 F = 0.60, n=1.00	
{5 }	O3P + NO2	--->	NO	k< 5> = 5.500E-12 * exp(188.0/T)	
{6 }	O3P + NO2	--->	NO3	k< 6> is a falloff expression using: ko = 2.500E-31 * (T/300)**(-1.80) kinf = 2.200E-11 * (T/300)**(-0.70) F = 0.60, n=1.00	
{7 }	O3 + NO	--->	NO2	k< 7> = 3.000E-12 * exp(-1500.0/T)	
{8 }	O3 + NO2	--->	NO3	k< 8> = 1.400E-13 * exp(-2470.0/T)	
{9 }	NO + NO3	--->	2.000*NO2	k< 9> = 1.800E-11 * exp(110.0/T)	
{10 }	NO + NO + O2	--->	2.000*NO2	k< 10> = 3.300E-39 * exp(530.0/T)	
{11 }	NO2 + NO3	--->	N2O5	k< 11> is a falloff expression using: ko = 3.600E-30 * (T/300)**(-4.10) kinf = 1.900E-12 * (T/300)**(0.20) F = 0.35, n=1.33	
{12 }	N2O5	--->	NO2 + NO3	k< 12> is a falloff expression using: ko = 1.300E-03 * (T/300)**(-3.50) * exp(-11000.0/T) kinf = 9.700E+14 * (T/300)**(0.10) * exp(-11080.0/T) F = 0.35, n=1.33	
{13 }	N2O5 + H2O	--->	2.000*HNO3	k< 13> = 1.000E-22	
{14 }	N2O5 + 2*H2O	--->	2.000*HNO3	k< 14> = 0.000E+00	
{15 }	NO2 + NO3	--->	NO + NO2	k< 15> = 4.500E-14 * exp(-1260.0/T)	
{16 }	NO3	--hv->	NO	NO3NO_06	See Table S-4
{17 }	NO3	--hv->	NO2 + O3P	NO3NO2_06	See Table S-4
{18 }	O3	--hv->	O1D	O3O1D_06	See Table S-4
{19 }	O3	--hv->	O3P	O3O3P_06	See Table S-4
{20 }	O1D + H2O	--->	2.000*OH	k< 20> = 1.630E-10 * exp(60.0/T)	
{21 }	O1D + M	--->	O3P	k< 21> = 2.380E-11 * exp(96.0/T)	
{22 }	OH + NO	--->	HONO	k< 22> is a falloff expression using: ko = 7.000E-31 * (T/300)**(-2.60)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
				kinf = 3.600E-11 * (T/300)**(-0.10) F = 0.60, n=1.00	
{23 }	HONO	--hv->	OH + NO	HONO_06	See Table S-4
{24 }	OH + HONO	--->	NO2	k< 24> = 2.500E-12 * exp(260.0/T)	
{25 }	OH + NO2	--->	HNO3	k< 25> is a falloff expression using: ko = 1.800E-30 * (T/300)**(-3.00) kinf = 2.800E-11 F = 0.60, n=1.00	
{26 }	OH + NO3	--->	HO2 + NO2	k< 26> = 2.000E-11	
{27 }	OH + HNO3	--->	NO3	k< 27> is a special rate expression of the form: k = ko + {k3[M] / (1 + k3[M]/k2)} ko = 2.400E-14 * exp(460.0/T) k2 = 2.700E-17 * exp(2199.0/T) k3 = 6.500E-34 * exp(1335.0/T)	
{28 }	HNO3	--hv->	OH + NO2	HNO3	See Table S-4
{29 }	OH + CO	--->	HO2 + CO2	k< 29> is a special rate expression of the form: k = k1 + k2[M] k1 = 1.440E-13 * exp(0.0/T) k2 = 3.430E-33 * exp(0.0/T)	
{30 }	OH + O3	--->	HO2	k< 30> = 1.700E-12 * exp(-940.0/T)	
{31 }	HO2 + NO	--->	OH + NO2	k< 31> = 3.600E-12 * exp(270.0/T)	
{32 }	HO2 + NO2	--->	HNO4	k< 32> is a falloff expression using: ko = 2.000E-31 * (T/300)**(-3.40) kinf = 2.900E-12 * (T/300)**(-1.10) F = 0.60, n=1.00	
{33 }	HNO4	--->	HO2 + NO2	k< 33> is a falloff expression using: ko = 3.720E-05 * (T/300)**(-2.40) * exp(-10650.0/T) kinf = 5.420E+15 * (T/300)**(-2.30) * exp(-11170.0/T) F = 0.60, n=1.00	
{34 }	HNO4	--hv->	0.610*HO2 +0.610*NO2 +0.390*OH +0.39*NO3	HNO4_06	See Table S-4
{35 }	HNO4 + OH	--->	NO2	k< 35> = 1.300E-12 * exp(380.0/T)	
{36 }	HO2 + O3	--->	OH	k< 36> = 2.030E-16 * (T/300)**(4.57) * exp(693.0/T)	
{37 }	HO2 + HO2	--->	HO2H	k< 37> is a special rate expression of the form: k = k1 + k2[M] k1 = 2.200E-13 * exp(600.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
			k2 = 1.900E-33 * exp(980.0/T)	
{38 }	HO2 + HO2 + H2O --->	HO2H	k< 38> is a special rate expression of the form: k = k1 + k2[M] k1 = 3.080E-34 * exp(2800.0/T) k2 = 2.660E-54 * exp(3180.0/T)	
{39 }	NO3 + HO2 --->	0.800*OH +0.800*NO2 +0.200*HNO3	k< 39> = 4.000E-12	
{40 }	NO3 + NO3 --->	2.000*NO2	k< 40> = 8.500E-13 * exp(-2450.0/T)	
{41 }	HO2H --hv->	2.000*OH	H2O2	See Table S-4
{42 }	HO2H + OH --->	HO2	k< 42> = 1.800E-12	
{43 }	OH + HO2 --->		k< 43> = 4.800E-11 * exp(250.0/T)	
{44 }	OH + SO2 --->	HO2 + SULF + SULRXN	k< 44> is a falloff expression using: ko = 3.300E-31 * (T/300)**(-4.30) kinf = 1.600E-12 F = 0.60, n=1.00	
{45 }	OH + H2 --->	HO2	k< 45> = 7.700E-12 * exp(-2100.0/T)	
{EX1 }	NO2 --hv->	NO2EX	NO2EX	See Table S-4
{EX2 }	NO2EX + M --->	NO2	k< 47> = 2.760E-11	
{EX3 }	NO2EX + H2O --->	NO2	k< 48> = 1.700E-10	
{EXOH}	NO2EX + H2O --->	OH + HONO	k< 49> = 0.000E+00	
{BR01}	MEO2 + NO --->	NO2 + HCHO + HO2	k< 50> = 2.300E-12 * exp(360.0/T)	
{BR02}	MEO2 + HO2 --->	COOH	k< 51> = 3.460E-13 * (T/300)**(0.36) * exp(780.0/T)	
{BR03}	MEO2 + HO2 --->	HCHO	k< 52> = 3.340E-14 * (T/300)**(-3.53) * exp(780.0/T)	
{BR04}	MEO2 + NO3 --->	HCHO + HO2 + NO2	k< 53> = 1.300E-12	
{BR05}	MEO2 + MEO2 --->	MEOH + HCHO	k< 54> = 6.390E-14 * (T/300)**(-1.80) * exp(365.0/T)	
{BR06}	MEO2 + MEO2 --->	2.000*HCHO +2.000*HO2	k< 55> = 7.400E-13 * exp(-520.0/T)	
{BR07}	RO2C + NO --->	NO2	k< 56> = 2.600E-12 * exp(380.0/T)	
{BR08}	RO2C + HO2 --->		k< 57> = 3.800E-13 * exp(900.0/T)	
{BR09}	RO2C + NO3 --->	NO2	k< 58> = 2.300E-12	
{BR10}	RO2C + MEO2 --->	0.500*HO2 +0.750*HCHO +0.250*MEOH	k< 59> = 2.000E-13	
{BR11}	RO2C + RO2C --->		k< 60> = 3.500E-14	
{BR12}	RO2XC + NO --->		k< 61> = 1.000E+00 * k(BR07)	
{BR13}	RO2XC + HO2 --->		k< 62> = 1.000E+00 * k(BR08)	
{BR14}	RO2XC + NO3 --->	NO2	k< 63> = 1.000E+00 * k(BR09)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{BR15}	RO2XC + MEO2	--->	0.500*HO2 +0.750*HCHO +0.250*MEOH	k< 64> = 1.000E+00 * k(BR10)	
{BR16}	RO2XC + RO2C	--->		k< 65> = 1.000E+00 * k(BR11)	
{BR17}	RO2XC + RO2XC	--->		k< 66> = 1.000E+00 * k(BR11)	
{BR18}	MECO3 + NO2	--->	PAN	k< 67> is a falloff expression using: ko = 2.700E-28 * (T/300)**(-7.10) kinf = 1.210E-11 * (T/300)**(-0.90) F = 0.30, n=1.41	
{BR19}	PAN	--->	MECO3 + NO2	k< 68> is a falloff expression using: ko = 4.900E-03 * exp(-12100.0/T) kinf = 4.000E+16 * exp(-13600.0/T) F = 0.30, n=1.41	
{BR20}	PAN	--hv->	0.600*MECO3 +0.600*NO2 +0.400*MEO2 + 0.4*CO2 +0.4*NO3	PAN	See Table S-4
{BR21}	MECO3 + NO	--->	MEO2 + CO2 + NO2	k< 70> = 7.500E-12 * exp(290.0/T)	
{BR22}	MECO3 + HO2	--->	0.700*CCOOOH +0.300*CCOOH +0.300*O3	k< 71> = 5.200E-13 * exp(980.0/T)	
{BR23}	MECO3 + NO3	--->	MEO2 + CO2 + NO2	k< 72> = 1.000E+00 * k(BR09)	
{BR24}	MECO3 + MEO2	--->	0.100*CCOOH +0.100*HCHO +0.900*HCHO +0.9*HO2 +0.9*MEO2 +0.9*CO2	k< 73> = 2.000E-12 * exp(500.0/T)	
{BR25}	MECO3 + RO2C	--->	MEO2 + CO2	k< 74> = 4.400E-13 * exp(1070.0/T)	
{BR26}	MECO3 + RO2XC	--->	MEO2 + CO2	k< 75> = 1.000E+00 * k(BR25)	
{BR27}	MECO3 + MECO3	--->	2.000*MEO2 +2.000*CO2	k< 76> = 2.900E-12 * exp(500.0/T)	
{BR28}	RCO3 + NO2	--->	PAN2	k< 77> = 1.210E-11 * (T/300)**(-1.07)	
{BR29}	PAN2	--->	RCO3 + NO2	k< 78> = 8.300E+16 * exp(-13940.0/T)	
{BR30}	PAN2	--hv->	0.600*RCO3 +0.600*NO2 +0.400*RO2C +0.4*xHO2 +0.4*yROOH +0.4*xCCHO +0.4*CO2 +0.4*NO3	PAN	See Table S-4
{BR31}	RCO3 + NO	--->	NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2	k< 80> = 6.700E-12 * exp(340.0/T)	
{BR32}	RCO3 + HO2	--->	0.750*RCOOOH +0.250*RCOOH +0.250*O3	k< 81> = 1.000E+00 * k(BR22)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{BR33}	RCO3 + NO3	--->	NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2	k< 82> = 1.000E+00 * k(BR09)	
{BR34}	RCO3 + MEO2	--->	HCHO + HO2 + RO2C + xHO2 + xCCHO + yROOH + CO2	k< 83> = 1.000E+00 * k(BR24)	
{BR35}	RCO3 + RO2C	--->	RO2C + xHO2 + xCCHO + yROOH + CO2	k< 84> = 1.000E+00 * k(BR25)	
{BR36}	RCO3 + RO2XC	--->	RO2C + xHO2 + xCCHO + yROOH + CO2	k< 85> = 1.000E+00 * k(BR25)	
{BR37}	RCO3 + MECO3	--->	2.000*CO2 + MEO2 + RO2C + xHO2 + yROOH + xCCHO	k< 86> = 1.000E+00 * k(BR27)	
{BR38}	RCO3 + RCO3	--->	2.000*RO2C +2.000*xHO2 +2.000*xCCHO +2.000*yROOH +2*CO2	k< 87> = 1.000E+00 * k(BR27)	
{BR39}	BZCO3 + NO2	--->	PBZN	k< 88> = 1.370E-11	
{BR40}	PBZN	--->	BZCO3 + NO2	k< 89> = 7.900E+16 * exp(-14000.0/T)	
{BR41}	PBZN	--hv->	0.600*BZCO3 +0.600*NO2 +0.400*CO2 +0.4*BZO +0.4*RO2C +0.4*NO3	PAN	See Table S-4
{BR42}	BZCO3 + NO	--->	NO2 + CO2 + BZO + RO2C	k< 91> = 1.000E+00 * k(BR31)	
{BR43}	BZCO3 + HO2	--->	0.750*RCOOOH +0.250*RCOOH +0.250*O3	k< 92> = 1.000E+00 * k(BR22)	
{BR44}	BZCO3 + NO3	--->	NO2 + CO2 + BZO + RO2C	k< 93> = 1.000E+00 * k(BR09)	
{BR45}	BZCO3 + MEO2	--->	HCHO + HO2 + RO2C + BZO + CO2	k< 94> = 1.000E+00 * k(BR24)	
{BR46}	BZCO3 + RO2C	--->	RO2C + BZO + CO2	k< 95> = 1.000E+00 * k(BR25)	
{BR47}	BZCO3 + RO2XC	--->	RO2C + BZO + CO2	k< 96> = 1.000E+00 * k(BR25)	
{BR48}	BZCO3 + MECO3	--->	2.000*CO2 + MEO2 + BZO + RO2C	k< 97> = 1.000E+00 * k(BR27)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{BR49}	BZCO3 + RCO3	--->	2.000*CO2 + RO2C + xHO2 + yROOH + xCCHO + BZO + RO2C	k< 98> = 1.000E+00 * k(BR27)	See Table S-4
{BR50}	BZCO3 + BZCO3	--->	2.000*BZO +2.000*RO2C +2.000*CO2	k< 99> = 1.000E+00 * k(BR27)	
{BR51}	MACO3 + NO2	--->	MAPAN	k<100> = 1.000E+00 * k(BR28)	
{BR52}	MAPAN	--->	MACO3 + NO2	k<101> = 1.600E+16 * exp(-13486.0/T)	
{BR53}	MAPAN	--hv->	0.600*MACO3 +0.600*NO2 +0.400*CO2 +0.4*HCHO +0.4*MECO3 +0.4*NO3	PAN	
{BR54}	MACO3 + NO	--->	NO2 + CO2 + HCHO + MECO3	k<103> = 1.000E+00 * k(BR31)	
{BR55}	MACO3 + HO2	--->	0.750*RCOOOH +0.250*RCOOH +0.250*O3	k<104> = 1.000E+00 * k(BR22)	
{BR56}	MACO3 + NO3	--->	NO2 + CO2 + HCHO + MECO3	k<105> = 1.000E+00 * k(BR09)	
{BR57}	MACO3 + MEO2	--->	2.000*HCHO + HO2 + CO2 + MECO3	k<106> = 1.000E+00 * k(BR24)	
{BR58}	MACO3 + RO2C	--->	CO2 + HCHO + MECO3	k<107> = 1.000E+00 * k(BR25)	
{BR59}	MACO3 + RO2XC	--->	CO2 + HCHO + MECO3	k<108> = 1.000E+00 * k(BR25)	
{BR60}	MACO3 + MECO3	--->	2.000*CO2 + MEO2 + HCHO + MECO3	k<109> = 1.000E+00 * k(BR27)	
{BR61}	MACO3 + RCO3	--->	HCHO + MECO3 + RO2C + xHO2 + yROOH + xCCHO 2*CO2	k<110> = 1.000E+00 * k(BR27)	
{BR62}	MACO3 + BZCO3	--->	HCHO + MECO3 + BZO + RO2C +2*CO2	k<111> = 1.000E+00 * k(BR27)	
{BR63}	MACO3 + MACO3	--->	2.000*HCHO +2.000*MECO3 +2.000*CO2	k<112> = 1.000E+00 * k(BR27)	
{BR64}	TBUO + NO2	--->	RNO3	k<113> = 2.400E-11	
{BR65}	TBUO	--->	ACETONE + MEO2	k<114> = 7.500E+14 * exp(-8152.0/T)	
{BR66}	BZO + NO2	--->	NPHE	k<115> = 2.300E-11 * exp(150.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{BR67}	BZO + HO2	--->	CRES	k<116> = 1.000E+00 * k(BR08)	
{BR68}	BZO	--->	CRES + RO2C + xHO2	k<117> = 1.000E-03	
{RO01}	xHO2	--->	HO2	k is variable parameter: RO2RO	See Table S-3
{RO02}	xHO2	--->		k is variable parameter: RO2XRO	See Table S-3
{RO03}	xOH	--->	OH	k is variable parameter: RO2RO	See Table S-3
{RO04}	xOH	--->		k is variable parameter: RO2XRO	See Table S-3
{RO05}	xNO2	--->	NO2	k is variable parameter: RO2RO	See Table S-3
{RO06}	xNO2	--->		k is variable parameter: RO2XRO	See Table S-3
{RO07}	xMEO2	--->	MEO2	k is variable parameter: RO2RO	See Table S-3
{RO08}	xMEO2	--->		k is variable parameter: RO2XRO	See Table S-3
{RO09}	xMECO3	--->	MECO3	k is variable parameter: RO2RO	See Table S-3
{RO10}	xMECO3	--->		k is variable parameter: RO2XRO	See Table S-3
{RO11}	xRCO3	--->	RCO3	k is variable parameter: RO2RO	See Table S-3
{RO12}	xRCO3	--->		k is variable parameter: RO2XRO	See Table S-3
{RO13}	xMACO3	--->	MACO3	k is variable parameter: RO2RO	See Table S-3
{RO14}	xMACO3	--->		k is variable parameter: RO2XRO	See Table S-3
{RO15}	xTBUO	--->	TBUO	k is variable parameter: RO2RO	See Table S-3
{RO16}	xTBUO	--->		k is variable parameter: RO2XRO	See Table S-3
{RO17}	xCO	--->	CO	k is variable parameter: RO2RO	See Table S-3
{RO18}	xCO	--->		k is variable parameter: RO2XRO	See Table S-3
{BP01}	HCHO	--hv->	2.000*HO2 + CO	HCHOR_06	See Table S-4
{BP02}	HCHO	--hv->	CO	HCHOM_06	See Table S-4
{BP03}	HCHO + OH	--->	HO2 + CO	k<147> = 5.400E-12 * exp(135.0/T)	
{BP07}	HCHO + NO3	--->	HNO3 + HO2 + CO	k<148> = 2.000E-12 * exp(-2431.0/T)	
{BP08}	CCHO + OH	--->	MECO3	k<149> = 4.400E-12 * exp(365.0/T)	
{BP09}	CCHO	--hv->	CO + HO2 + MEO2	CCHO_R	See Table S-4
{BP10}	CCHO + NO3	--->	HNO3 + MECO3	k<151> = 1.400E-12 * exp(-1860.0/T)	
{BP11}	RCHO + OH	--->	0.965*RCO3 +0.035*RO2C +0.035*xHO2 +0.035*xCO +0.035*xCCHO +0.035*yROOH	k<152> = 5.100E-12 * exp(405.0/T)	
{BP12}	RCHO	--hv->	RO2C + xHO2 + yROOH + xCCHO + CO + HO2	C2CHO	See Table S-4
{BP13}	RCHO + NO3	--->	HNO3 + RCO3	k<154> = 1.400E-12 * exp(-1601.0/T)	
{BP14}	ACETONE + OH	--->	RO2C + xMECO3 + xHCHO	k<155> = 4.560E-14 * (T/300)**(3.65) * exp(429.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
			+ yROOH		
{BP15}	ACETONE	--hv->	0.620*MECO3 +1.380*MEO2 +0.380*CO	ACET_06	See Table S-4
{BP16}	MEK + OH	--->	0.967*RO2C +0.039*RO2XC +0.039*zRNO3 +0.376*xHO2 +0.51*xMECO3 +0.074*xRCO3 +0.088*xHCHO +0.504*xCCHO +0.376*xRCHO + yROOH	k<157> = 1.300E-12 * (T/300)**(2.00) * exp(-25.0/T)	
{BP17}	MEK	--hv->	MECO3 + RO2C + xHO2 + xCCHO + yROOH		See Table S-4
{BP18}	MEOH + OH	--->	HCHO + HO2	k<159> = 2.850E-12 * exp(-345.0/T)	
{BP19}	HCOOH + OH	--->	HO2 + CO2	k<160> = 4.500E-13	
{BP20}	CCOOH + OH	--->	0.509*MEO2 +0.491*RO2C +0.509*CO2 +0.491*xHO2 +0.491*xMGLY +0.491*yROOH	k<161> = 4.200E-14 * exp(855.0/T)	
{BP21}	RCOOH + OH	--->	RO2C + xHO2 +0.143*CO2 +0.142*xCCHO +0.4*xRCHO +0.457*xBACL + yROOH - 0.455*XC	k<162> = 1.200E-12	
{BP22}	COOH + OH	--->	0.300*HCHO +0.300*OH +0.700*MEO2	k<163> = 3.800E-12 * exp(200.0/T)	
{BP23}	COOH	--hv->	HCHO + HO2 + OH	COOH	See Table S-4
{BP24}	ROOH + OH	--->	0.744*OH +0.251*RO2C +0.004*RO2XC +0.004*zRNO3 +0.744*RCHO +0.239*xHO2 +0.012*xOH +0.012*xHCHO +0.012*xCCHO +0.205*xRCHO +0.034*xPROD2 +0.256*yROOH	k<165> = 2.500E-11	
{BP25}	ROOH	--hv->	RCHO + HO2 + OH	COOH	See Table S-4
{BP26}	R6OOH + OH	--->	0.840*OH +0.222*RO2C +0.029*RO2XC +0.029*zRNO3 +0.84*PRD2 +0.09*xHO2	k<167> = 5.600E-11	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
			+0.041*xOH +0.02*xCCHO +0.075*xRCHO +0.084*xPROD2 +0.16*yROOH		
{BP27}	R6OOH	--hv->	OH +0.142*HO2 +0.782*RO2C +0.077*RO2XC +0.077*zRNO3 +0.085*RCHO +0.142*PRD2 +0.782*xHO2 +0.026*xCCHO +0.058*xRCHO +0.698*xPROD2 +0.858*yR6OOH	COOH	See Table S-4
{BP28}	RAOOH + OH	--->	0.139*OH +0.148*HO2 +0.589*RO2C +0.124*RO2XC +0.124*zRNO3 +0.074*PRD2 +0.147*MGLY +0.139*IPRD +0.565*xHO2 +0.024*xOH +0.448*xRCHO +0.026*xGLY +0.03*xMEK +0.252*xMGLY +0.073*xAFG1 +0.073*xAFG2 +0.713*yR6OOH	k<169> = 1.410E-10	
{BP29}	RAOOH	--hv->	OH + HO2 +0.500*GLY +0.5*MGLY +0.5*AFG1 +0.5*AFG2	COOH	See Table S-4
{BP30}	GLY	--hv->	2.000*CO +2.000*HO2	GLY_07R	See Table S-4
{BP31}	GLY	--hv->	HCHO + CO	GLY_07M	See Table S-4
{BP32}	GLY + OH	--->	0.630*HO2 +1.260*CO +0.370*RCO3	k<173> = 1.100E-11	
{BP33}	GLY + NO3	--->	HNO3 +0.630*HO2 +1.260*CO +0.37*RCO3	k<174> = 2.800E-12 * exp(-2376.0/T)	
{BP34}	MGLY	--hv->	HO2 + CO + MECO3	MGLY_06	See Table S-4
{BP35}	MGLY + OH	--->	CO + MECO3	k<176> = 1.500E-11	
{BP36}	MGLY + NO3	--->	HNO3 + CO + MECO3	k<177> = 1.400E-12 * exp(-1895.0/T)	
{BP37}	BACL	--hv->	2.000*MECO3	BACL_07	See Table S-4
{BP38}	CRES + OH	--->	0.200*BZO +0.800*RO2C +0.800*xHO2 +0.8*yR6OOH +0.25*xMGLY	k<179> = 1.700E-12 * exp(950.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{BP39}	CRES + NO3	--->	HNO3 + BZO	k<180> = 1.400E-11	
{BP40}	NPHE + OH	--->	BZO	k<181> = 3.500E-12	
{BP41}	NPHE	--hv->	HONO	1.500E-03 * NO2_06	See Table S-4
{BP42}	NPHE	--hv->		1.500E-02 * NO2_06	See Table S-4
{BP43}	BALD + OH	--->	BZCO3	k<184> = 1.200E-11	
{BP44}	BALD	--hv->		6.000E-02 * BALD_06	See Table S-4
{BP45}	BALD + NO3	--->	HNO3 + BZCO3	k<186> = 1.340E-12 * exp(-1860.0/T)	
{BP46}	AFG1 + OH	--->	0.217*MACO3 +0.723*RO2C +0.060*RO2XC +0.06*zRNO3 +0.521*xHO2 +0.201*xMECO3 +0.334*xCO +0.407*xRCHO +0.129*xMEK +0.107*xGLY +0.267*xMGLY +0.783*yR6OOH	k<187> = 7.400E-11	
{BP47}	AFG1 + O3	--->	0.826*OH +0.522*HO2 +0.652*RO2C +0.522*CO +0.174*CO2 +0.432*GLY +0.568*MGLY +0.652*xRCO3 +0.652*xHCHO +0.652*yR6OOH	k<188> = 9.660E-18	
{BP48}	AFG1	--hv->	1.023*HO2 +0.173*MEO2 +0.305*MECO3 +0.5*MACO3 +0.695*CO +0.195*GLY +0.305*MGLY	AFG1	See Table S-4
{BP49}	AFG2 + OH	--->	0.217*MACO3 +0.723*RO2C +0.060*RO2XC +0.06*zRNO3 +0.521*xHO2 +0.201*xMECO3 +0.334*xCO +0.407*xRCHO +0.129*xMEK +0.107*xGLY +0.267*xMGLY +0.783*yR6OOH	k<190> = 7.400E-11	
{BP50}	AFG2 + O3	--->	0.826*OH +0.522*HO2 +0.652*RO2C +0.522*CO +0.174*CO2 +0.432*GLY	k<191> = 9.660E-18	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants			products	rate expression	Notes
				+0.568*MGLY +0.652*xRCO3 +0.652*xHCHO +0.652*yR6OOH		
{BP51}	AFG2		--hv->	PRD2 AFG1		See Table S-4
{BP52}	AFG3	+ OH	--->	0.206*MACO3 +0.733*RO2C +0.117*RO2XC +0.117*zRNO3 +0.561*xHO2 +0.117*xMECO3 +0.114*xCO +0.274*xGLY +0.153*xMGLY +0.019*xBACL +0.195*xAFG1 +0.195*xAFG2 +0.231*xIPRD +0.794*yR6OOH	k<193> = 9.350E-11	
{BP53}	AFG3	+ O3	--->	0.471*OH +0.554*HO2 +0.013*MECO3 +0.258*RO2C +0.007*RO2XC +0.007*zRNO3 +0.58*CO +0.19*CO2 +0.366*GLY +0.184*MGLY +0.35*AFG1 +0.35*AFG2 +0.139*AFG3 +0.003*MACR +0.004*MVK +0.003*IPRD +0.095*xHO2 +0.163*xRCO3	k<194> = 1.430E-17	
{BP54}	MACR	+ OH	--->	0.500*MACO3 +0.500*RO2C +0.500*xHO2 +0.416*xCO +0.084*xHCHO +0.416*xMEK +0.084*xMGLY +0.5*yROOH	k<195> = 8.000E-12 * exp(380.0/T)	
{BP55}	MACR	+ O3	--->	0.208*OH +0.108*HO2 +0.100*RO2C +0.45*CO +0.117*CO2 +0.1*HCHO +0.9*MGLY +0.333*HCOOH +0.1*xRCO3 +0.1*xHCHO +0.1*yROOH	k<196> = 1.400E-15 * exp(-2100.0/T)	
{BP56}	MACR	+ NO3	--->	0.500*MACO3 +0.500*RO2C +0.500*HNO3	k<197> = 1.500E-12 * exp(-1815.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
			+0.5*xHO2 +0.5*xCO +0.5*yROOH		
{BP57}	MACR + O3P	--->	RCHO	k<198> = 6.340E-12	
{BP58}	MACR	--hv->	0.330*OH +0.670*HO2 +0.340*MECO3 +0.33*MACO3 +0.33*RO2C +0.67*CO +0.34*HCHO +0.33*xMECO3 +0.33*xHCHO +0.33*yROOH	MACR_06	See Table S-4
{BP59}	MVK + OH	--->	0.975*RO2C +0.025*RO2XC +0.025*zRNO3 +0.3*xHO2 +0.675*xMECO3 +0.3*xHCHO +0.675*xHOCCHO +0.3*xMGLY + yROOH	k<200> = 2.600E-12 * exp(610.0/T)	
{BP60}	MVK + O3	--->	0.164*OH +0.064*HO2 +0.050*RO2C +0.05*xHO2 +0.475*CO +0.124*CO2 +0.05*HCHO +0.95*MGLY +0.351*HCOOH +0.05*xRCO3 +0.05*xHCHO +0.05*yROOH	k<201> = 8.500E-16 * exp(-1520.0/T)	
{BP62}	MVK + O3P	--->	0.450*RCHO +0.550*MEK	k<202> = 4.320E-12	
{BP63}	MVK	--hv->	0.400*MEO2 +0.600*CO +0.600*PRD2 +0.4*MACO3	MVK_06	See Table S-4
{BP64}	IPRD + OH	--->	0.289*MACO3 +0.670*RO2C +0.670*xHO2 +0.041*RO2XC +0.041*zRNO3 +0.336*xCO +0.055*xHCHO +0.129*xHOCCHO +0.013*xRCHO +0.15*xMEK +0.332*xPROD2 +0.15*xGLY +0.174*xMGLY +0.711*yR6OOH	k<204> = 6.190E-11	
{BP65}	IPRD + O3	--->	0.285*OH +0.400*HO2 +0.048*RO2C	k<205> = 4.180E-18	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.048*xRCO3 +0.498*CO +0.14*CO2 +0.124*HCHO +0.21*MEK +0.023*GLY +0.742*MGLY +0.1*HCOOH +0.372*RCOOH +0.047*xHOCCHO +0.001*xHCHO +0.048*yR6OOH		
{BP66}	IPRD + NO3 --->	0.150*MACO3 +0.150*HNO3 +0.799*RO2C +0.799*xHO2 +0.051*RO2XC +0.051*zRNO3 +0.572*xCO +0.227*xHCHO +0.218*xRCHO +0.008*xMGLY +0.572*xRNO3 +0.85*yR6OOH	k<206> = 1.000E-13	
{BP67}	IPRD --hv->	1.233*HO2 +0.467*MECO3 +0.300*RCO3 +1.233*CO +0.3*HCHO +0.467*HOCCHO +0.233*MEK	MACR_06	See Table S-4
{BP68}	PRD2 + OH --->	0.472*HO2 +0.379*xHO2 +0.029*xMECO3 +0.049*xRCO3 +0.473*RO2C +0.071*RO2XC +0.071*zRNO3 +0.002*HCHO +0.211*xHCHO +0.001*CCHO +0.083*xCCHO +0.143*RCHO +0.402*xRCHO +0.115*xMEK +0.329*PRD2 +0.007*xPROD2 +0.528*yR6OOH	k<208> = 1.550E-11	
{BP69}	PRD2 --hv->	0.913*xHO2 +0.400*MECO3 +0.600*RCO3 +1.59*RO2C +0.087*RO2XC +0.087*zRNO3 +0.303*xHCHO +0.163*xCCHO +0.78*xRCHO + yR6OOH	4.860E-03*MEK_06	See Table S-4

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{BP70}	RNO3 + OH	--->	0.189*HO2 +0.305*xHO2 +0.019*NO2 +0.313*xNO2 +0.976*RO2C +0.175*RO2XC +0.175*zRNO3 +0.011*xHCHO +0.429*xCCHO +0.001*RCHO +0.036*xRCHO +0.004*xACETONE +0.01*MEK +0.17*xMEK +0.008*PRD2 +0.031*xPROD2 +0.189*RNO3 +0.305*xRNO3	k<210> = 7.200E-12	
{BP71}	RNO3	--hv->	0.344*HO2 +0.554*xHO2 + NO2 +0.721*RO2C +0.102*RO2XC +0.102*zRNO3 +0.074*HCHO +0.061*xHCHO +0.214*CCHO +0.23*xCCHO +0.074*RCHO +0.063*xRCHO +0.008*xACETONE +0.124*MEK +0.083*xMEK +0.19*PRD2 +0.261*xPROD2 +0.066*yROOH	IC3ONO2	See Table S-4
{BP72}	HOCCHO + OH	--->	MECO3	k<212> = 1.000E+00 * k(BP08)	
{BP73}	HOCCHO	--hv->	CO +2.000*HO2 + HCHO	HOCCHO_IUPAC	See Table S-4
{BP74}	HOCCHO + NO3	--->	HNO3 + MECO3	k<214> = 1.000E+00 * k(BP10)	
{BP75}	ACROLEIN + OH	--->	0.250*xHO2 +0.750*MACO3 +0.250*RO2C +0.167*xCO +0.083*xHCHO +0.167*xCCHO +0.083*xGLY +0.25*yROOH - 0.75*XC	k<215> = 1.990E-11	
{BP76}	ACROLEIN + O3	--->	0.830*HO2 +0.330*OH +1.005*CO +0.31*CO2 +0.5*HCHO +0.185*HCOOH +0.5*GLY	k<216> = 1.400E-15 * exp(-2528.0/T)	
{BP77}	ACROLEIN + NO3	--->	0.031*xHO2 +0.967*MACO3 +0.031*RO2C	k<217> = 1.180E-15	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
			+0.002*RO2XC +0.002*zRNO3 +0.967*HNO3 +0.031*xCO +0.031*xRNO3 +0.033*yROOH		
{BP78}	ACROLEIN + O3P	--->	RCHO	k<218> = 2.370E-12	
{BP79}	ACROLEIN	--hv->	1.066*HO2 +0.178*OH +0.234*MEO2 +0.33*MACO3 +1.188*CO +0.102*CO2 +0.34*HCHO +0.05*CCOOH - 0.284*XC	ACRO_09	See Table S-4
{BP80}	CCOOOH + OH	--->	0.980*MECO3 +0.020*RO2C +0.020*CO2 +0.02*xOH +0.02*xHCHO +0.02*yROOH	k<220> = 5.280E-12	
{BP81}	CCOOOH	--hv->	MEO2 + CO2 + OH	PAA	See Table S-4
{BP82}	RCOOOH + OH	--->	0.806*RCO3 +0.194*RO2C +0.194*yROOH +0.11*CO2 +0.11*xOH +0.11*xCCHO +0.084*xHO2 +0.084*xRCHO	k<222> = 6.420E-12	
{BP83}	RCOOOH	--hv->	xHO2 + xCCHO + yROOH + CO2 + OH	PAA	See Table S-4
{PO01}	xHCHO	--->	HCHO	k is variable parameter: RO2RO	See Table S-3
{PO02}	xHCHO	--->		k is variable parameter: RO2XRO	See Table S-3
{PO03}	xCCHO	--->	CCHO	k is variable parameter: RO2RO	See Table S-3
{PO04}	xCCHO	--->		k is variable parameter: RO2XRO	See Table S-3
{PO05}	xRCHO	--->	RCHO	k is variable parameter: RO2RO	See Table S-3
{PO06}	xRCHO	--->		k is variable parameter: RO2XRO	See Table S-3
{PO07}	xACETONE	--->	ACETONE	k is variable parameter: RO2RO	See Table S-3
{PO08}	xACETONE	--->		k is variable parameter: RO2XRO	See Table S-3
{PO09}	xMEK	--->	MEK	k is variable parameter: RO2RO	See Table S-3
{PO10}	xMEK	--->		k is variable parameter: RO2XRO	See Table S-3
{PO11}	xPROD2	--->	PRD2	k is variable parameter: RO2RO	See Table S-3
{PO12}	xPROD2	--->		k is variable parameter: RO2XRO	See Table S-3
{PO13}	xGLY	--->	GLY	k is variable parameter: RO2RO	See Table S-3
{PO14}	xGLY	--->		k is variable parameter: RO2XRO	See Table S-3

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{PO15}	xMGLY	--->	MGLY	k is variable parameter: RO2RO	See Table S-3
{PO16}	xMGLY	--->		k is variable parameter: RO2XRO	See Table S-3
{PO17}	xBACL	--->	BACL	k is variable parameter: RO2RO	See Table S-3
{PO18}	xBACL	--->		k is variable parameter: RO2XRO	See Table S-3
{PO19}	xBALD	--->	BALD	k is variable parameter: RO2RO	See Table S-3
{PO20}	xBALD	--->		k is variable parameter: RO2XRO	See Table S-3
{PO21}	xAFG1	--->	AFG1	k is variable parameter: RO2RO	See Table S-3
{PO22}	xAFG1	--->		k is variable parameter: RO2XRO	See Table S-3
{PO23}	xAFG2	--->	AFG2	k is variable parameter: RO2RO	See Table S-3
{PO24}	xAFG2	--->		k is variable parameter: RO2XRO	See Table S-3
{PO25}	xAFG3	--->	AFG3	k is variable parameter: RO2RO	See Table S-3
{PO26}	xAFG3	--->		k is variable parameter: RO2XRO	See Table S-3
{PO27}	xMACR	--->	MACR	k is variable parameter: RO2RO	See Table S-3
{PO28}	xMACR	--->		k is variable parameter: RO2XRO	See Table S-3
{PO29}	xMVK	--->	MVK	k is variable parameter: RO2RO	See Table S-3
{PO30}	xMVK	--->		k is variable parameter: RO2XRO	See Table S-3
{PO31}	xIPRD	--->	IPRD	k is variable parameter: RO2RO	See Table S-3
{PO32}	xIPRD	--->		k is variable parameter: RO2XRO	See Table S-3
{PO33}	xRNO3	--->	RNO3	k is variable parameter: RO2RO	See Table S-3
{PO34}	xRNO3	--->		k is variable parameter: RO2XRO	See Table S-3
{PO35}	zRNO3	--->	RNO3	k is variable parameter: RO2NO	See Table S-3
{PO36}	zRNO3	--->	PRD2 + HO2	k is variable parameter: RO22NN	See Table S-3
{PO37}	zRNO3	--->		k is variable parameter: RO2XRO	See Table S-3
{PO38}	yROOH	--->	ROOH	k is variable parameter: RO2HO2	See Table S-3
{PO39}	yROOH	--->	MEK	k is variable parameter: RO2RO2M	See Table S-3
{PO40}	yROOH	--->		k is variable parameter: RO2RO	See Table S-3
{PO41}	yR6OOH	--->	R6OOH	k is variable parameter: RO2HO2	See Table S-3
{PO42}	yR6OOH	--->	PRD2	k is variable parameter: RO2RO2M	See Table S-3
{PO43}	yR6OOH	--->		k is variable parameter: RO2RO	See Table S-3
{PO44}	yRAOOH	--->	RAOOH	k is variable parameter: RO2HO2	See Table S-3
{PO45}	yRAOOH	--->	PRD2	k is variable parameter: RO2RO2M	See Table S-3
{PO46}	yRAOOH	--->		k is variable parameter: RO2RO	See Table S-3
{PO47}	xHOCCHO	--->	HOCCHO	k is variable parameter: RO2RO	See Table S-3
{PO48}	xHOCCHO	--->		k is variable parameter: RO2XRO	See Table S-3
{PO49}	xACROLEIN	--->	ACROLEIN	k is variable parameter: RO2RO	See Table S-3
{PO50}	xACROLEIN	--->		k is variable parameter: RO2XRO	See Table S-3

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{BE01}	CH4 + OH	--->	MEO2	k<274> = 1.850E-12 * exp(-1690.0/T)	
{BE02}	ETHENE + OH	--->	xHO2 + RO2C +1.610*xHCHO +0.195*xHOCCHO + yROOH	k<275> is a falloff expression using: ko = 1.000E-28 * (T/300)**(-4.50) kinf = 8.800E-12 * (T/300)**(-0.85) F = 0.60, n=1.00	
{BE03}	ETHENE + O3	--->	0.160*HO2 +0.160*OH +0.510*CO +0.12*CO2 + HCHO +0.37*HCOOH	k<276> = 9.140E-15 * exp(-2580.0/T)	
{BE04}	ETHENE + NO3	--->	xHO2 + RO2C + xRCHO + yROOH	k<277> = 3.300E-12 * (T/300)**(2.00) * exp(-2880.0/T)	
{BE05}	ETHENE + O3P	--->	0.800*HO2 +0.290*xHO2 +0.510*MEO2 +0.29*RO2C +0.51*CO +0.278*xCO +0.278*xHCHO +0.1*CCHO +0.012*xGLY +0.29*yROOH	k<278> = 1.070E-11 * exp(-800.0/T)	
{BT01}	PROPENE + OH	--->	0.984*xHO2 +0.984*RO2C +0.016*RO2XC +0.016*zRNO3 +0.984*xHCHO +0.984*xCCHO + yROOH	k<279> = 4.850E-12 * exp(504.0/T)	
{BT02}	PROPENE + O3	--->	0.165*HO2 +0.350*OH +0.355*MEO2 +0.525*CO +0.215*CO2 +0.5*HCHO +0.5*CCHO +0.185*HCOOH +0.075*CCOOH	k<280> = 5.510E-15 * exp(-1878.0/T)	
{BT03}	PROPENE + NO3	--->	0.949*xHO2 +0.949*RO2C +0.051*RO2XC +0.051*zRNO3 + yROOH	k<281> = 4.590E-13 * exp(-1156.0/T)	
{BT04}	PROPENE + O3P	--->	0.450*RCHO +0.550*MEK	k<282> = 1.020E-11 * exp(-280.0/T)	
{BT05}	BUTADIENE13 + OH	--->	0.951*xHO2 +1.189*RO2C +0.049*RO2XC +0.049*zRNO3 +0.708*xHCHO +0.48*xACROLEIN +0.471*xIPRD + yROOH	k<283> = 1.480E-11 * exp(448.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
{BT06}	BUTADIENE13 + O3 --->	0.080*HO2 +0.080*OH +0.255*CO +0.185*CO2 +0.5*HCHO +0.185*HCOOH +0.5*ACROLEIN +0.375*MVK +0.125*PRD2	k<284> = 1.340E-14 * exp(-2283.0/T)	
{BT07}	BUTADIENE13 + NO3 --->	0.815*xHO2 +0.120*xNO2 +1.055*RO2C +0.065*RO2XC +0.065*zRNO3 +0.115*xHCHO +0.46*xMVK +0.12*xIPRD +0.355*xRNO3 + yROOH	k<285> = 1.000E-13	
{BT08}	BUTADIENE13 + O3P --->	0.250*HO2 +0.117*xHO2 +0.118*xMACO3 +0.235*RO2C +0.015*RO2XC +0.015*zRNO3 +0.115*xCO +0.115*xACROLEIN +0.001*xAFG1 +0.001*xAFG2 +0.75*PRD2 +0.25*yROOH	k<286> = 2.260E-11 * exp(-40.0/T)	
{BE06}	ISOPRENE + OH --->	0.907*xHO2 +0.986*RO2C +0.093*RO2XC +0.093*zRNO3 +0.624*xHCHO +0.23*xMACR +0.32*xMVK +0.357*xIPRD + yR6OOH + ISOPRXN	k<287> = 2.540E-11 * exp(410.0/T)	
{BE07}	ISOPRENE + O3 --->	0.066*HO2 +0.266*OH +0.192*xMACO3 +0.192*RO2C +0.008*RO2XC +0.008*zRNO3 +0.275*CO +0.122*CO2 +0.4*HCHO +0.192*xHCHO +0.204*HCOOH +0.39*MACR +0.16*MVK +0.15*IPRD +0.1*PRD2 +0.2*yR6OOH	k<288> = 7.860E-15 * exp(-1912.0/T)	
{BE08}	ISOPRENE + NO3 --->	0.749*xHO2 +0.187*xNO2 +0.936*RO2C	k<289> = 3.030E-12 * exp(-448.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.064*RO2XC +0.064*zRNO3 +0.936*xIPRD + yR6OOH		
{BE09}	ISOPRENE + O3P --->	0.250*MEO2 +0.240*xMACO3 +0.240*RO2C +0.01*RO2XC +0.01*zRNO3 +0.24*xHCHO +0.75*PRD2 +0.25*yR6OOH	k<290> = 3.500E-11	
{BT09}	APIN + OH --->	0.799*xHO2 +0.004*xRCO3 +1.042*RO2C +0.197*RO2XC +0.197*zRNO3 +0.002*xCO +0.022*xHCHO +0.776*xRCHO +0.034*xACETONE +0.02*xMGLY +0.023*xBACL + yR6OOH + TRPRXN	k<291> = 1.210E-11 * exp(436.0/T)	
{BT10}	APIN + O3 --->	0.009*HO2 +0.102*xHO2 +0.728*OH +0.001*xMECO3 +0.297*xRCO3 +1.511*RO2C +0.337*RO2XC +0.337*zRNO3 +0.029*CO +0.051*xCO +0.017*CO2 +0.344*xHCHO +0.24*xRCHO +0.345*xACETONE +0.008*MEK +0.002*xGLY +0.081*xBACL +0.255*PRD2	k<292> = 5.000E-16 * exp(-530.0/T)	
{BT11}	APIN + NO3 --->	0.056*xHO2 +0.643*xNO2 +0.007*xRCO3 +1.05*RO2C +0.293*RO2XC +0.293*zRNO3 +0.005*xCO +0.007*xHCHO +0.684*xRCHO +0.069*xACETONE +0.002*xMGLY +0.056*xRNO3 + yR6OOH + TRPRXN	k<293> = 1.190E-12 * exp(490.0/T)	
{BT12}	APIN + O3P --->	PRD2 + TRPRXN	k<294> = 3.200E-11	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
{BE10}	ACETYLENE + OH --->	0.300*HO2 +0.700*OH +0.300*CO +0.3*HCOOH +0.7*GLY	k<295> is a falloff expression using: ko = 5.500E-30 * (T/300)**(-2.00) kinf = 8.300E-13 F = 0.60, n=1.00	
{BE11}	ACETYLENE + O3 --->	1.500*HO2 +0.500*OH +1.500*CO +0.5*CO2	k<296> = 1.000E-14 * exp(-4100.0/T)	
{BE12}	BENZENE + OH --->	0.570*HO2 +0.290*xHO2 +0.116*OH +0.29*RO2C +0.024*RO2XC +0.024*zRNO3 +0.29*xGLY +0.57*CRES +0.029*xAFG1 +0.261*xAFG2 +0.116*AFG3 +0.314*yRAOOH + BENZRO2	k<297> = 2.330E-12 * exp(-193.0/T)	
{BT13}	TOLUENE + OH --->	0.181*HO2 +0.454*xHO2 +0.312*OH +0.454*RO2C +0.054*RO2XC +0.054*zRNO3 +0.238*xGLY +0.151*xMGLY +0.181*CRES +0.065*xBALD +0.195*xAFG1 +0.195*xAFG2 +0.312*AFG3 +0.073*yR6OOH +0.435*yRAOOH + TOLRO2	k<298> = 1.810E-12 * exp(338.0/T)	
{BT14}	MXYL + OH --->	0.159*HO2 +0.520*xHO2 +0.239*OH +0.52*RO2C +0.082*RO2XC +0.082*zRNO3 +0.1*xGLY +0.38*xMGLY +0.159*CRES +0.041*xBALD +0.336*xAFG1 +0.144*xAFG2 +0.239*AFG3 +0.047*yR6OOH +0.555*yRAOOH + XYLRO2	k<299> = 2.310E-11	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
{BT15}	OXYL + OH --->	0.161*HO2 +0.554*xHO2 +0.198*OH +0.554*RO2C +0.087*RO2XC +0.087*zRNO3 +0.084*xGLY +0.238*xMGLY +0.185*xBACL +0.161*CRES +0.047*xBALD +0.253*xAFG1 +0.253*xAFG2 +0.198*AFG3 +0.055*yR6OOH +0.586*yRAOOH + XYLRO2	k<300> = 1.360E-11	
{BT16}	PXYL + OH --->	0.159*HO2 +0.487*xHO2 +0.278*OH +0.487*RO2C +0.076*RO2XC +0.076*zRNO3 +0.286*xGLY +0.112*xMGLY +0.159*CRES +0.088*xBALD +0.045*xAFG1 +0.067*xAFG2 +0.278*AFG3 +0.286*xAFG3 +0.102*yR6OOH +0.461*yRAOOH + XYLRO2	k<301> = 1.430E-11	
{BT17}	TRIMETH_BENZ + OH --->	0.022*HO2 +0.627*xHO2 +0.230*OH +0.627*RO2C +0.121*RO2XC +0.121*zRNO3 +0.074*xGLY +0.405*xMGLY +0.112*xBACL +0.022*CRES +0.036*xBALD +0.088*xAFG1 +0.352*xAFG2 +0.23*AFG3 +0.151*xAFG3 +0.043*yR6OOH +0.705*yRAOOH + XYLRO2	k<302> = 3.250E-11	
{BT18}	ETOH + OH --->	0.950*HO2 +0.050*xHO2 +0.050*RO2C +0.081*xHCHO +0.95*CCHO +0.01*xHOCCHO +0.05*yROOH	k<303> = 5.490E-13 * (T/300)**(2.00) * exp(530.0/T)	
{BL01}	ALK1 + OH --->	xHO2 + RO2C + xCCHO	k<304> = 1.340E-12 * (T/300)**(2.00) * exp(-499.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+ yROOH		
{BL02}	ALK2 + OH --->	0.965*xHO2 +0.965*RO2C +0.035*RO2XC +0.035*zRNO3 +0.261*xRCHO +0.704*xACETONE + yROOH	k<305> = 1.490E-12 * (T/300)**(2.00) * exp(-87.0/T)	
{BL03}	ALK3 + OH --->	0.695*xHO2 +0.236*xTBUO +1.253*RO2C +0.07*RO2XC +0.07*zRNO3 +0.026*xHCHO +0.445*xCCHO +0.122*xRCHO +0.024*xACETONE +0.332*xMEK +0.983*yROOH +0.017*yR6OOH	k<306> = 1.510E-12 * exp(126.0/T)	
{BL04}	ALK4 + OH --->	0.830*xHO2 +0.010*xMEO2 +0.011*xMECO3 +1.763*RO2C +0.149*RO2XC +0.149*zRNO3 +0.002*xCO +0.029*xHCHO +0.438*xCCHO +0.236*xRCHO +0.426*xACETONE +0.106*xMEK +0.146*xPROD2 + yR6OOH	k<307> = 3.750E-12 * exp(44.0/T)	
{BL05}	ALK5 + OH --->	0.647*xHO2 +1.605*RO2C +0.353*RO2XC +0.353*zRNO3 +0.04*xHCHO +0.106*xCCHO +0.209*xRCHO +0.071*xACETONE +0.086*xMEK +0.407*xPROD2 + yR6OOH + ALK5RXN	k<308> = 2.700E-12 * exp(374.0/T)	
{BL06}	OLE1 + OH --->	0.871*xHO2 +0.001*xMEO2 +1.202*RO2C +0.128*RO2XC +0.128*zRNO3 +0.582*xHCHO +0.01*xCCHO +0.007*xHOCCHO +0.666*xRCHO +0.007*xACETONE +0.036*xACROLEIN +0.001*xMACR	k<309> = 6.720E-12 * exp(501.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants			products	rate expression	Notes
				+0.012*xMVK +0.009*xIPRD +0.168*xPROD2 +0.169*yROOH +0.831*yR6OOH		
{BL07}	OLE1	+ O3	--->	0.095*HO2 +0.057*xHO2 +0.128*OH +0.09*RO2C +0.005*RO2XC +0.005*zRNO3 +0.303*CO +0.088*CO2 +0.5*HCHO +0.011*xCCHO +0.5*RCHO +0.044*xRCHO +0.003*xACETONE +0.009*MEK +0.185*HCOOH +0.159*RCOOH +0.268*PRD2 +0.011*yROOH	k<310> = 3.190E-15 * exp(-1701.0/T)	
{BL08}	OLE1	+ NO3	--->	0.772*xHO2 +1.463*RO2C +0.228*RO2XC +0.228*zRNO3 +0.013*xCCHO +0.003*xRCHO +0.034*xACETONE +0.774*xRNO3 +0.169*yROOH +0.831*yR6OOH	k<311> = 5.370E-13 * exp(-1047.0/T)	
{BL09}	OLE1	+ O3P	--->	0.450*RCHO +0.390*MEK +0.160*PRD2	k<312> = 1.610E-11 * exp(-326.0/T)	
{BL10}	OLE2	+ OH	--->	0.912*xHO2 +0.953*RO2C +0.088*RO2XC +0.088*zRNO3 +0.179*xHCHO +0.835*xCCHO +0.51*xRCHO +0.144*xACETONE +0.08*xMEK +0.002*xMVK +0.012*xIPRD +0.023*xPROD2 +0.319*yROOH +0.681*yR6OOH	k<313> = 1.260E-11 * exp(488.0/T)	
{BL11}	OLE2	+ O3	--->	0.094*HO2 +0.041*xHO2 +0.443*OH +0.307*MEO2 +0.156*xMECO3 +0.008*xRCO3 +0.212*RO2C +0.003*RO2XC +0.003*zRNO3	k<314> = 8.590E-15 * exp(-1255.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.299*CO +0.161*CO2 +0.131*HCHO +0.114*xHCHO +0.453*CCHO +0.071*xCCHO +0.333*RCHO +0.019*xRCHO +0.051*ACETONE		
{BL12}	OLE2 + NO3 --->	0.400*xHO2 +0.426*xNO2 +0.035*xMEO2 +1.193*RO2C +0.14*RO2XC +0.14*zRNO3 +0.072*xHCHO +0.579*xCCHO +0.163*xRCHO +0.116*xACETONE +0.002*xMEK +0.32*xRNO3 +0.319*yROOH +0.681*yR6OOH	k<315> = 2.310E-13 * exp(382.0/T)	
{BL13}	OLE2 + O3P --->	0.079*RCHO +0.751*MEK +0.170*PRD2	k<316> = 1.430E-11 * exp(111.0/T)	
{BL14}	ARO1 + OH --->	0.123*HO2 +0.566*xHO2 +0.202*OH +0.566*RO2C +0.11*RO2XC +0.11*zRNO3 +0.158*xGLY +0.1*xMGLY +0.123*CRES +0.072*xAFG1 +0.185*xAFG2 +0.202*AFG3 +0.309*xPROD2 +0.369*yR6OOH + TOLRO2	k<317> = 7.840E-12	
{BL15}	ARO2 + OH --->	0.077*HO2 +0.617*xHO2 +0.178*OH +0.617*RO2C +0.128*RO2XC +0.128*zRNO3 +0.088*xGLY +0.312*xMGLY +0.134*xBACL +0.077*CRES +0.026*xBALD +0.221*xAFG1 +0.247*xAFG2 +0.178*AFG3 +0.068*xAFG3 +0.057*xPROD2 +0.101*yR6OOH + XYLRO2	k<318> = 3.090E-11	
{BL16}	TERP + OH --->	0.734*xHO2 +0.064*xRCO3 +1.211*RO2C	k<319> = 2.270E-11 * exp(435.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.201*RO2XC +0.201*zRNO3 +0.001*xCO +0.411*xHCHO +0.385*xRCHO +0.037*xACETONE +0.007*xMEK +0.003*xMGLY +0.009*xBACL +0.003*xMVK +0.002*xIPRD +0.409*xPROD2 + yR6OOH + TRPRXN		
{BL17}	TERP + O3 --->	0.078*HO2 +0.046*xHO2 +0.499*OH +0.202*xMECO3 +0.059*xRCO3 +0.49*RO2C +0.121*RO2XC +0.121*zRNO3 +0.249*CO +0.063*CO2 +0.127*HCHO +0.033*xHCHO +0.208*xRCHO +0.057*xACETONE +0.002*MEK +0.172*HCOOH +0.068*RCOOH +0.003*xMGLY	k<320> = 8.280E-16 * exp(-785.0/T)	
{BL18}	TERP + NO3 --->	0.227*xHO2 +0.287*xNO2 +0.026*xRCO3 +1.786*RO2C +0.46*RO2XC +0.46*zRNO3 +0.012*xCO +0.023*xHCHO +0.002*xHOCCHO +0.403*xRCHO +0.239*xACETONE +0.005*xMACR +0.001*xMVK +0.004*xIPRD +0.228*xRNO3 + yR6OOH + TRPRXN	k<321> = 1.330E-12 * exp(490.0/T)	
{BL19}	TERP + O3P --->	0.237*RCHO +0.763*PRD2 + TRPRXN	k<322> = 4.020E-11	
{BT19}	SESQ + OH --->	0.734*xHO2 +0.064*xRCO3 +1.211*RO2C +0.201*RO2XC +0.201*zRNO3 +0.001*xCO +0.411*xHCHO +0.385*xRCHO +0.037*xACETONE	k<323> = 1.000E+00 * k(BL16)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.007*xMEK +0.003*xMGLY +0.009*xBACL +0.003*xMVK +0.002*xIPRD +0.409*xPROD2 + yR6OOH + SESQRXN		
{BT20}	SESQ + O3 --->	0.078*HO2 +0.046*xHO2 +0.499*OH +0.202*xMECO3 +0.059*xRCO3 +0.49*RO2C +0.121*RO2XC +0.121*zRNO3 +0.249*CO +0.063*CO2 +0.127*HCHO +0.033*xHCHO +0.208*xRCHO +0.057*xACETONE +0.002*MEK +0.172*HCOOH +0.068*RCOOH +0.003*xMGLY	k<324> = 1.000E+00 * k(BL17)	
{BT21}	SESQ + NO3 --->	0.227*xHO2 +0.287*xNO2 +0.026*xRCO3 +1.786*RO2C +0.46*RO2XC +0.46*zRNO3 +0.012*xCO +0.023*xHCHO +0.002*xCCHO +0.403*xRCHO +0.239*xACETONE +0.005*xMACR +0.001*xMVK +0.004*xIPRD +0.228*xRNO3 + yR6OOH + SESQRXN	k<325> = 1.000E+00 * k(BL18)	
{BT22}	SESQ + O3P --->	0.237*RCHO +0.763*PRD2 + SESQRXN	k<326> = 1.000E+00 * k(BL19)	
{CI01}	CL2 --hv->	2.000*CL	CL2	See Table S-4
{CI02}	CL + NO + M --->	CLNO	k<328> = 7.600E-32 * (T/300)**(-1.80)	
{CI03}	CLNO --hv->	CL + NO	CLNO_06	See Table S-4
{CI04}	CL + NO2 --->	CLONO	k<330> is a falloff expression using: ko = 1.300E-30 * (T/300)**(-2.00) kinf = 1.000E-10 * (T/300)**(-1.00) F = 0.60, n=1.00	
{CI05}	CL + NO2 --->	CLNO2	k<331> is a falloff expression using: ko = 1.800E-31 * (T/300)**(-2.00)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
				kinf = 1.000E-10 * (T/300)**(-1.00) F = 0.60, n=1.00	
{CI06}	CLONO	--hv->	CL + NO2	CLONO	See Table S-4
{CI07}	CLNO2	--hv->	CL + NO2	CLNO2	See Table S-4
{CI08}	CL + HO2	--->	HCL	k<334> = 3.440E-11 * (T/300)**(-0.56)	
{CI09}	CL + HO2	--->	CLO + OH	k<335> = 9.410E-12 * (T/300)**(2.10)	
{CI10}	CL + O3	--->	CLO	k<336> = 2.800E-11 * exp(-250.0/T)	
{CI11}	CL + NO3	--->	CLO + NO2	k<337> = 2.400E-11	
{CI12}	CLO + NO	--->	CL + NO2	k<338> = 6.200E-12 * exp(295.0/T)	
{CI13}	CLO + NO2	--->	CLONO2	k<339> is a falloff expression using: ko = 1.800E-31 * (T/300)**(-3.40) kinf = 1.500E-11 * (T/300)**(-1.90) F = 0.60, n=1.00	
{CI14}	CLONO2	--hv->	CLO + NO2	CLONO2_1	See Table S-4
{CI15}	CLONO2	--hv->	CL + NO3	CLONO2_2	See Table S-4
{CI16}	CLONO2	--->	CLO + NO2	k<342> is a falloff expression using: ko = 4.480E-05 * (T/300)**(-1.00) * exp(-12530.0/T) kinf = 3.710E+15 * (T/300)**(3.50) * exp(-12530.0/T) F = 0.60, n=1.00	
{CI17}	CL + CLONO2	--->	CL2 + NO3	k<343> = 6.200E-12 * exp(145.0/T)	
{CI18}	CLO + HO2	--->	HOCL	k<344> = 2.200E-12 * exp(340.0/T)	
{CI19}	HOCL	--hv->	OH + CL	HOCL_06	See Table S-4
{CI20}	CLO + CLO	--->	0.290*CL2 +1.420*CL	k<346> = 1.250E-11 * exp(-1960.0/T)	
{CI21}	OH + HCL	--->	CL	k<347> = 1.700E-12 * exp(-230.0/T)	
{CI22}	CL + H2	--->	HCL + HO2	k<348> = 3.900E-11 * exp(-2310.0/T)	
{CP01}	HCHO + CL	--->	HCL + HO2 + CO	k<349> = 8.100E-11 * exp(-30.0/T)	
{CP02}	CCHO + CL	--->	HCL + MECO3	k<350> = 8.000E-11	
{CP03}	MEOH + CL	--->	HCL + HCHO + HO2	k<351> = 5.500E-11	
{CP04}	RCHO + CL	--->	HCL +0.900*RCO3 +0.100*RO2C +0.1*xCCHO +0.1*xCO +0.1*xHO2 +0.1*yROOH	k<352> = 1.230E-10	
{CP05}	ACETONE + CL	--->	HCL + RO2C + xHCHO + xMECO3 + yROOH	k<353> = 7.700E-11 * exp(-1000.0/T)	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{CP06}	MEK + CL	--->	HCL +0.975*RO2C +0.039*RO2XC +0.039*zRNO3 +0.84*xHO2 +0.085*xMECO3 +0.036*xRCO3 +0.065*xHCHO +0.07*xCCHO +0.84*xRCHO + yROOH	k<354> = 3.600E-11	
{CP07}	RNO3 + CL	--->	HCL +0.038*NO2 +0.055*HO2 +1.282*RO2C +0.202*RO2XC +0.202*zRNO3 +0.009*RCHO +0.018*MEK +0.012*PRD2 +0.055*RNO3 +0.159*xNO2 +0.547*xHO2 +0.045*xHCHO +0.3*xCCHO +0.02*xRCHO +0.003*xACETONE +0.041*xMEK +0.046*xPROD2	k<355> = 1.920E-10	
{CP08}	PRD2 + CL	--->	HCL +0.314*HO2 +0.680*RO2C +0.116*RO2XC +0.116*zRNO3 +0.198*RCHO +0.116*PRD2 +0.541*xHO2 +0.007*xMECO3 +0.022*xRCO3 +0.237*xHCHO +0.109*xCCHO +0.591*xRCHO +0.051*xMEK +0.04*xPROD2 +0.686*yR6OOH	k<356> = 2.000E-10	
{CP09}	GLY + CL	--->	HCL +0.630*HO2 +1.260*CO +0.37*RCO3	k<357> = 8.100E-11 * exp(-30.0/T)	
{CP10}	MGLY + CL	--->	HCL + CO + MECO3	k<358> = 8.000E-11	
{CP11}	CRES + CL	--->	HCL + xHO2 + xBALD + yR6OOH	k<359> = 6.200E-11	
{CP12}	BALD + CL	--->	HCL + BZCO3	k<360> = 8.000E-11	
{CP13}	ROOH + CL	--->	HCL +0.414*OH +0.588*RO2C	k<361> = 1.660E-10	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.414*RCHO +0.104*xOH +0.482*xHO2 +0.106*xHCHO +0.104*xCCHO +0.197*xRCHO +0.285*xMEK +0.586*yROOH		
{CP14}	R6OOH + CL --->	HCL +0.145*OH +1.078*RO2C +0.117*RO2XC +0.117*zRNO3 +0.145*PRD2 +0.502*xOH +0.237*xHO2 +0.186*xCCHO +0.676*xRCHO +0.28*xPROD2 +0.855*yR6OOH	k<362> = 3.000E-10	
{CP15}	RAOOH + CL --->	0.404*HCL +0.139*OH +0.148*HO2 +0.589*RO2C +0.124*RO2XC +0.124*zRNO3 +0.074*PRD2 +0.147*MGLY +0.139*IPRD +0.565*xHO2 +0.024*xOH +0.448*xRCHO +0.026*xGLY +0.03*xMEK +0.252*xMGLY +0.073*xAFG1 +0.073*xAFG2 +0.713*yR6OOH	k<363> = 4.290E-10	
{TP01}	ACROLEIN + CL --->	0.484*xHO2 +0.274*xCL +0.216*MACO3 +1.032*RO2C +0.026*RO2XC +0.026*zRNO3 +0.216*HCL +0.484*xCO +0.274*xHCHO +0.274*xGLY +0.484*xCLCCHO +0.784*yROOH	k<364> = 2.940E-10	
{CP16}	MACR + CL --->	0.250*HCL +0.165*MACO3 +0.802*RO2C +0.033*RO2XC +0.033*zRNO3 +0.802*xHO2 +0.541*xCO +0.082*xIPRD +0.18*xCLCCHO +0.541*xCLACET +0.835*yROOH	k<365> = 3.850E-10	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
{CP17}	MVK + CL --->	1.283*RO2C +0.053*RO2XC +0.053*zRNO3 +0.322*xHO2 +0.625*xMECO3 +0.947*xCLCCHO + yROOH	k<366> = 2.320E-10	
{CP18}	IPRD + CL --->	0.401*HCL +0.084*HO2 +0.154*MACO3 +0.73*RO2C +0.051*RO2XC +0.051*zRNO3 +0.042*AFG1 +0.042*AFG2 +0.712*xHO2 +0.498*xCO +0.195*xHCHO +0.017*xMGLY +0.009*xAFG1 +0.009*xAFG2 +0.115*xIPRD +0.14*xCLCCHO +0.42*xCLACET +0.762*yR6OOH	k<367> = 4.120E-10	
{CP19}	CLCCHO --hv->	HO2 + CO + RO2C + xCL + xHCHO + yROOH	CLCCHO	See Table S-4
{CP20}	CLCCHO + OH --->	RCO3	k<369> = 3.100E-12	
{CP21}	CLCCHO + CL --->	HCL + RCO3	k<370> = 1.290E-11	
{CP22}	CLACET --hv->	MECO3 + RO2C + xCL + xHCHO + yROOH	5.000E-01 * CLACET	See Table S-4
{CP23}	xCL --->	CL	k is variable parameter: RO2RO	See Table S-3
{CP24}	xCL --->		k is variable parameter: RO2XRO	See Table S-3
{CP25}	xCLCCHO --->	CLCCHO	k is variable parameter: RO2RO	See Table S-3
{CP26}	xCLCCHO --->		k is variable parameter: RO2XRO	See Table S-3
{CP27}	xCLACET --->	CLACET	k is variable parameter: RO2RO	See Table S-3
{CP28}	xCLACET --->		k is variable parameter: RO2XRO	See Table S-3
{CE01}	CH4 + CL --->	HCL + MEO2	k<378> = 7.300E-12 * exp(-1280.0/T)	
{CE02}	ETHENE + CL --->	xHO2 +2.000*RO2C + xHCHO + CLCHO	k<379> is a falloff expression using: ko = 1.600E-29 * (T/300)**(-3.30) kinf = 3.100E-10 * (T/300)**(-1.00) F = 0.60, n=1.00	
{TE01}	PROPENE + CL --->	0.124*HCL +0.971*xHO2 +0.971*RO2C	k<380> = 2.670E-10	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.029*RO2XC +0.029*zRNO3 +0.124*xACROLEIN +0.306*xCLCCHO +0.54*xCLACET + yROOH		
{TE02}	BUTADIENE13 + CL --->	0.390*xHO2 +0.541*xCL +1.884*RO2C +0.069*RO2XC +0.069*zRNO3 +0.863*xHCHO +0.457*xACROLEIN +0.473*xIPRD + yROOH	k<381> = 4.900E-10	
{CE03}	ISOPRENE + CL --->	0.150*HCL +0.738*xHO2 +0.177*xCL +1.168*RO2C +0.085*RO2XC +0.085*zRNO3 +0.275*xHCHO +0.177*xMVK +0.671*xIPRD +0.067*xCLCCHO + yR6OOH	k<382> = 4.800E-10	
{TE03}	APIN + CL --->	0.548*HCL +0.252*xHO2 +0.068*xCL +0.034*xMECO3 +0.05*xRCO3 +0.016*xMACO3 +2.258*RO2C +0.582*RO2XC +0.582*zRNO3 +0.035*xCO +0.158*xHCHO +0.185*xRCHO +0.274*xACETONE +0.007*xGLY +0.003*xBACL +0.003*xMVK +0.158*xIPRD +0.006*xAFG1	k<383> = 5.460E-10	
{CE04}	ACETYLENE + CL --->	HO2 + CO	k<384> is a falloff expression using: ko = 5.200E-30 * (T/300)**(-2.40) kinf = 2.200E-10 F = 0.60, n=1.00	
{TE04}	TOLUENE + CL --->	0.894*xHO2 +0.894*RO2C +0.106*RO2XC +0.106*zRNO3 +0.894*xBALD	k<385> = 6.200E-11	
{TE05}	MXYL + CL --->	0.864*xHO2 +0.864*RO2C +0.136*RO2XC +0.136*zRNO3 +0.864*xBALD	k<386> = 1.350E-10	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants		products	rate expression	Notes
{TE06}	OXYL + CL	--->	0.864*xHO2 +0.864*RO2C +0.136*RO2XC +0.136*zRNO3 +0.864*xBALD	k<387> = 1.400E-10	
{TE07}	PXYL + CL	--->	0.864*xHO2 +0.864*RO2C +0.136*RO2XC +0.136*zRNO3 +0.864*xBALD	k<388> = 1.440E-10	
{TE08}	TRIMETH_BENZ + CL	--->	0.838*xHO2 +0.838*RO2C +0.162*RO2XC +0.162*zRNO3 +0.838*xBALD	k<389> = 2.420E-10	
{TE09}	ETOH + CL	--->	HCL +0.688*HO2 +0.312*xHO2 +0.312*RO2C +0.503*xHCHO +0.688*CCHO +0.061*xHOCCHO +0.312*yROOH	k<390> = 8.600E-11 * exp(45.0/T)	
{BC01}	ALK1 + CL	--->	HCL + xHO2 + RO2C + xCCHO + yROOH	k<391> = 8.300E-11 * exp(-100.0/T)	
{BC02}	ALK2 + CL	--->	HCL +0.970*xHO2 +0.970*RO2C +0.03*RO2XC +0.03*zRNO3 +0.482*xRCHO +0.488*xACETONE + yROOH	k<392> = 1.200E-10 * exp(40.0/T)	
{BC03}	ALK3 + CL	--->	HCL +0.835*xHO2 +0.094*xTBUO +1.361*RO2C +0.07*RO2XC +0.07*zRNO3 +0.078*xHCHO +0.34*xCCHO +0.343*xRCHO +0.075*xACETONE +0.253*xMEK +0.983*yROOH +0.017*yR6OOH	k<393> = 1.860E-10	
{BC04}	ALK4 + CL	--->	HCL +0.827*xHO2 +0.003*xMEO2 +0.004*xMECO3 +1.737*RO2C +0.165*RO2XC +0.165*zRNO3 +0.003*xCO +0.034*xHCHO +0.287*xCCHO +0.412*xRCHO +0.247*xACETONE	k<394> = 2.630E-10	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.076*xMEK +0.13*xPROD2 + yR6OOH		
{BC05}	ALK5 + CL --->	HCL +0.647*xHO2 +1.541*RO2C +0.352*RO2XC +0.352*zRNO3 +0.022*xHCHO +0.08*xCCHO +0.258*xRCHO +0.044*xACETONE +0.041*xMEK +0.378*xPROD2 + yR6OOH	k<395> = 4.210E-10	
{BC06}	OLE1 + CL --->	0.384*HCL +0.873*xHO2 +1.608*RO2C +0.127*RO2XC +0.127*zRNO3 +0.036*xHCHO +0.206*xCCHO +0.072*xRCHO +0.215*xACROLEIN +0.019*xMVK +0.038*xIPRD +0.192*xCLCCHO +0.337*xCLACET +0.169*yROOH +0.831*yR6OOH	k<396> = 3.920E-10	
{BC07}	OLE2 + CL --->	0.279*HCL +0.450*xHO2 +0.442*xCL +0.001*xMEO2 +1.492*RO2C +0.106*RO2XC +0.106*zRNO3 +0.19*xHCHO +0.383*xCCHO +0.317*xRCHO +0.086*xACETONE +0.042*xMEK +0.025*xMACR +0.058*xMVK +0.161*xIPRD +0.013*xCLCCHO +0.191*xCLACET +0.319*yROOH	k<397> = 3.770E-10	
{BC08}	ARO1 + CL --->	0.840*xHO2 +0.840*RO2C +0.160*RO2XC +0.16*zRNO3 +0.84*xPROD2	k<398> = 2.160E-10	
{BC09}	ARO2 + CL --->	0.828*xHO2 +0.828*RO2C +0.172*RO2XC +0.172*zRNO3 +0.469*xBALD +0.359*xPROD2	k<399> = 2.660E-10	
{BC10}	TERP + CL --->	0.548*HCL +0.252*xHO2 +0.068*xCL	k<400> = 5.460E-10	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
		+0.034*xMECO3 +0.05*xRCO3 +0.016*xMACO3 +2.258*RO2C +0.582*RO2XC +0.582*zRNO3 +0.035*xCO +0.158*xHCHO +0.185*xRCHO +0.274*xACETONE +0.007*xGLY +0.003*xBACL +0.003*xMVK +0.158*xIPRD +0.006*xAFG1		
{BC11}	SESQ + CL --->	0.252*xHO2 +0.068*xCL +0.034*xMECO3 +0.05*xRCO3 +0.016*xMACO3 +2.258*RO2C +0.582*RO2XC +0.582*zRNO3 +0.548*HCL +0.035*xCO +0.158*xHCHO +0.185*xRCHO +0.274*xACETONE +0.007*xGLY +0.003*xBACL +0.003*xMVK +0.158*xIPRD +0.006*xAFG1	k<401> = 1.000E+00 * k(BC10)	
{AE51}	BENZRO2 + NO --->	NO + BNZNRXN	k<402> = 1.000E+00 * k(BR07)	
{AE52}	BENZRO2 + HO2 --->	HO2 + BNZHRXN	k<403> = 1.000E+00 * k(BR08)	
{AE53}	XYLRO2 + NO --->	NO + XYLNRXN	k<404> = 1.000E+00 * k(BR07)	
{AE54}	XYLRO2 + HO2 --->	HO2 + XYLHRXN	k<405> = 1.000E+00 * k(BR08)	
{AE55}	TOLRO2 + NO --->	NO + TOLNRXN	k<406> = 1.000E+00 * k(BR07)	
{AE56}	TOLRO2 + HO2 --->	HO2 + TOLHRXN	k<407> = 1.000E+00 * k(BR08)	
{TR01}	HCHO_PRIMARY --hv->		HCHOR_06	See Table S-4
{TR02}	HCHO_PRIMARY --hv->		HCHOM_06	See Table S-4
{TR03}	HCHO_PRIMARY + OH --->	OH	k<410> = 5.400E-12 * exp(135.0/T)	
{TR05}	HCHO_PRIMARY + NO3 --->	NO3	k<411> = 2.000E-12 * exp(-2431.0/T)	
{TR06}	HCHO_PRIMARY + CL --->	CL	k<412> = 8.100E-11 * exp(-30.0/T)	
{TR07}	CCHO_PRIMARY + OH --->	OH	k<413> = 4.400E-12 * exp(365.0/T)	
{TR08}	CCHO_PRIMARY --hv->		CCHO_R	See Table S-4
{TR09}	CCHO_PRIMARY + NO3 --->	NO3	k<415> = 1.400E-12 * exp(-1860.0/T)	
{TR10}	CCHO_PRIMARY + CL --->	HCL	k<416> = 8.000E-11	

Table S-1
Reaction Listing for SAPRC07TB mechanism

name	reactants	products	rate expression	Notes
{TR11}	ACROLEIN_PRIMARY + OH	--->	k<417> = 1.990E-11	
{TR12}	ACROLEIN_PRIMARY+ O3	--->	k<418> = 1.400E-15 * exp(-2528.0/T)	
{TR13}	ACROLEIN_PRIMARY + NO3	--->	k<419> = 1.180E-15	
{TR14}	ACROLEIN_PRIMARY+ O3P	--->	k<420> = 2.370E-12	
{TR15}	ACROLEIN_PRIMARY	--hv->	ACRO_09	See Table S-4
{TR16}	ACROLEIN_PRIMARY+ CL	--->	k<422> = 2.940E-10	

1

Table S-2
SAPRC07TB Mechanism Species

Species	Definition	Molecular weight
ACETONE	Acetone	58.08
ACETYLENE	Acetylene	26.04
ACROLEIN	Acrolein	56.06
ACROLEIN_PRIMARY	Acrolein emissions tracer	56.06
AFG1	Lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form radicals	98.10
AFG2	Lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form non-radical products	98.10
AFG3	Lumped diunsaturatred dicarbonyl aromatic fragmentation product.	124.14
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2 and 5 x 10^2 ppm^{-1} min^{-1}. (Primarily ethane)	30.07
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^2 and 2.5 x 10^3 ppm^{-1} min^{-1}. (Primarily propane and acetylene)	36.73
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2.5 x 10^3 and 5 x 10^3 ppm^{-1} min^{-1}.	58.61
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 103 and 1 x 104 ppm-1 min-1.	77.6
ALK5	Alkanes and other non-aromatic compounds that react only with OH, and have kOH greater than 1 x 10^4 ppm^{-1} min^{-1}.	118.89

Table S-2
SAPRC07TB Mechanism Species

Species	Definition	Molecular weight
ALK5RXN	SOA precursor compounds products from largest alkanes (ALK5)	118.9
APIN	α-pinene	136.23
ARO1	Aromatics with kOH < $2x10^4$ ppm^{-1} min^{-1}.	95.16
ARO2	Aromatics with kOH > $2x10^4$ ppm^{-1} min^{-1}.	118.72
BACL	Biacetyl	86.09
BALD	Aromatic aldehydes (e.g., benzaldehyde)	106.13
BENZENE	Benzene	78.11
BNZHRXN	SOA precursor compounds from benzene via peroxy radical reaction with HO2	127
BNZNRXN	SOA precursor compounds from benzene via peroxy radical reaction with NO	127
BNZRO2	SOA precursor surrogate from benzene	127
BUTADIENE13	1,3-butadiene	54.09
BZCO3	Peroxyacyl radical formed from Aromatic Aldehydes	137.11
BZO	Phenoxy Radicals	93
CCHO	Acetaldehyde	44.05
CCHO_PRIMARY	Acetaldehyde Emissions Tracer	44.05
CCOOH	Acetic Acid. Also used for peroxyacetic acid in Carter	60.05
CCOOOH	Proposed for Peroxyacetic Acid	76
CH4	Methane, held constant	16.04
CL	Chlorine atoms	35.5
CL2	Chlorine molecules	70
CLACET	Chloroacetone (and other alpha-chloro ketones that are assumed to be similarly photoreactive)	92.5
CLCCHO	Chloroacetaldehyde (and other alpha-chloro aldehydes that are assumed to be similarly photoreactive)	78.5
CLCHO	Formyl Chloride (assumed to be unreactive)	64.5
CLNO	Nitrosyl Chloride	65.5

Table S-2
SAPRC07TB Mechanism Species

Species	Definition	Molecular weight
CLNO2	Nitryl Chloride	83.5
CLO	ClO. Radicals	51.5
CLONO	ClONO	81.5
CLONO2	ClONO2	96.5
CO	Carbon Monoxide	28.01
CO2	Carbon Dioxide	44.01
COOH	Methyl Hydroperoxide	48.04
CRES	Phenols and Cresols	108.14
ETHENE	Ethene	28.05
ETOH	Ethanol	46.068
GLY	Glyoxal	58.04
H2	Hydrogen Molecules	2.016
H2O	Water	18.02
HCHO	Formaldehyde	30.03
HCHO_PRIMARY	Formaldehyde Emission Tracer	30.03
HCL	Hydrochloric acid	36.5
HCOOH	Formic Acid	46.03
HNO3	Nitric Acid	63.02
HNO4	Peroxynitric Acid	79.02
HO2	Hydroperoxide Radicals	33.01
HO2H	Hydrogen Peroxide	34.01
HOCCHO	Glycolaldehyde	60.05
HOCL	HOCl	52.5
HOCOO	Radical formed when Formaldehyde reacts with HO2	51
HONO	Nitrous Acid	47.02
HV	Light	0
IPRD	Lumped isoprene product species	100.12
ISOPRENE	Isoprene	68.12
ISOPRXN	SOA precursor compounds from isoprene	68
M	Air	28.85
MACO3	Peroxyacyl radicals formed from methacrolein and other acroleins.	101.08
MACR	Methacrolein	70.09

Table S-2
SAPRC07TB Mechanism Species

Species	Definition	Molecular weight
MAPAN	PAN analogue formed from Methacrolein	147.09
MECO3	Acetyl Peroxy Radicals	75.04
MEK	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5 x 10-13 but slower than 5 x 10-12 cm3 molec-2 sec-1. (Based on mechanism for methyl ethyl ketone).	72.11
MEO2	Methyl Peroxy Radicals	47.03
MEOH	Methanol	32.04
MGLY	Methyl Glyoxal	72.07
MVK	Methyl Vinyl Ketone	70.09
MXYL	m-xylene	106.16
N2O5	Nitrogen Pentoxide	108.02
NO	Nitric Oxide	30.01
NO2	Nitrogen Dioxide	46.01
NO2EX	Electronically excited NO2 (only needed if reaction with H2O forming OH is non-negligible)	44
NO3	Nitrate Radical	62.01
NPHE	Nitrophenols	139.11
O1D	Excited Oxygen Atoms	16
O2	Oxygen	31.99
O3	Ozone	47.99
O3P	Ground State Oxygen Atoms	16
OH	Hydroxyl Radicals	17.01
OLE1	Alkenes (other than ethene) with kOH < 7x104 ppm-1 min-1.	72.34
OLE2	Alkenes with kOH > 7x104 ppm-1 min-1.	75.78
OXYL	o-xylene	106.16
PAN	Peroxy Acetyl Nitrate	121.05
PAN2	PPN and other higher alkyl PAN analogues	135.08
PBZN	PAN analogues formed from Aromatic Aldehydes	183.13

Table S-2
SAPRC07TB Mechanism Species

Species	Definition	Molecular weight
PRD2	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5 x 10-12 cm3 molec-2 sec-1.	116.16
PROPENE	propene	42.08
PXYL	p-xylene	106.16
R6OOH	Lumped organic hydroperoxides with 5 or more carbons (other than those formed following OH addition to aromatic rings, which is represented separately). Mechanism based on that estimated for 3-hexyl hydroperoxide.	118.17
RAOOH	Organic hydroperoxides formed following OH addition to aromatic rings, which is represented separately because of their probable role in SOA formation. Mechanism based on two isomers expected to be formed in the m-xylene system.	188.18
RCHO	Lumped C3+ Aldehydes (mechanism based on propionaldehyde)	58.08
RCO3	Peroxy Propionyl and higher peroxy acyl Radicals	89.07
RCOOH	Higher organic acids and, in Carter, peroxy acids (mechanism based on propionic acid).	74.08
RCOOOH	Proposed Higher organic peroxy acids	74.08
RNO3	Lumped Organic Nitrates	147.18
RO2C	Peroxy Radical Operator representing NO to NO2 and NO3 to NO2 conversions, and the effects of peroxy radical reactions on acyl peroxy and other peroxy radicals.	1

Table S-2
SAPRC07TB Mechanism Species

Species	Definition	Molecular weight
RO2XC	Peroxy Radical Operator representing NO consumption (used in conjunction with organic nitrate formation), and the effects of peroxy radical reactions on NO3, acyl peroxy radicals, and other peroxy radicals.	1
ROOH	Lumped organic hydroperoxides with 2-4 carbons. Mechanism based on that estimated for n-propyl hydroperoxide.	76.1
SESQ	Sesquiterpenes	204.35
SESQRXN	SOA precursor compounds from sesquiterpines	204
SO2	Sulfur Dioxide	64.06
SULF	Sulfates (SO3 or H2SO4)	98.08
SULRXN	Sulfate Aerosol Precursor	98.08
TBUO	t-Butoxy Radicals	73
TERP	Terpenes	136.24
TOLHRXN	SOA precursor compounds from toluene and less reactive aromatics (ARO1) via peroxy radical reaction with HO2	147.60
TOLNRXN	SOA precursor compounds from toluene and less reactive aromatics (ARO1) via peroxy radical reaction with NO	147.60
TOLRO2	SOA precursor surrogate from toluene and ARO1 reactions with OH	147.6
TOLUENE	toluene	92.14
TRIMETH_BENZ124	1,2,4-trimethyl benzene	120.19
TRPRXN	SOA precursor compounds from α-pinene and terpenes	136
xACETONE	As above, but for ACETONE	58.08
xACROLEIN	As above, but for ACROLEIN	56.06
xAFG1	As above, but for AFG1	98.1
xAFG2	As above, but for AFG2	98.1
xAFG3	As above, but for AFG3	124.74
xBACL	As above, but for BACL	86.09
xBALD	As above, but for BALD	106.13

Table S-2
SAPRC07TB Mechanism Species

Species	Definition	Molecular weight
xCCHO	As above, but for CCHO	44.05
xCL	Formation of Cl radicals from alkoxy radicals formed in peroxy radical reactions with NO and NO3 (100% yields) and RO2 (50% yields)	35.5
xCLACET	As above, but for CLACET	92.5
xCLCCHO	As above, but for CLCCHO	78.5
xCO	As above, but for CO	28.01
xGLY	As above, but for GLY	58.04
xHCHO	As above, but for HCHO	30.03
xHO2	Formation of HO2 from alkoxy radicals formed in peroxy radical reactions with NO and NO3 (100% yields) and RO2 (50% yields)	33.01
xHOCCHO	As above, but for HOCCHO	60.05
xIPRD	As above, but for IPRD	100.12
xMACO3	As above, but for MACO3	101.08
xMACR	As above, but for MACR	70.09
xMECO3	As above, but for MECO3	75.04
xMEK	As above, but for MEK	72.11
xMEO2	As above, but for MEO2	47.03
xMGLY	As above, but for MGLY	72.07
xMVK	As above, but for MVK	70.09
xNO2	As above, but for NO2	46.01
xOH	As above, but for OH	17.01
xPROD2	As above, but for PROD2	116.16
xRCHO	As above, but for RCHO	58.08
xRCO3	As above, but for RCO3	89.07
xRNO3	As above, but for RNO3	147.18
xTBUO	As above, but for TBUO	73
XYLHRXN	SOA precursor compounds from xylene and higher reactive aromatics (ARO2) via peroxy radical reaction with HO2	167.70

Table S-2
SAPRC07TB Mechanism Species

Species	Definition	Molecular weight
XYLNRXN	SOA precursor compounds from xylene and higher reactive aromatics (ARO2) via peroxy radical reaction with NO	167.70
XYLRO2	SOA precursor surrogate from xylene and ARO2 reactions with OH	167.20
yR6OOH	As above, but the RO2 + HO2 product is represented by R6OOH and the H-shift products are represented by PROD2.	118.17
yRAOOH	As above, but for RAOOH	188.18
yROOH	Formation of ROOH following RO2 + HO2 reactions, or formation of H-shift disproportionation products (represented by MEK) in the RO2 + RCO3 and (in 50% yields) RO2 + RO2 reactions.	76.1
zRNO3	Formation of RNO3 in the RO2 + NO, reaction, or formation of corresponding non-nitrate products (represented by PROD2) formed from alkoxy radicals formed in RO2 + NO3 and (in 50% yields) RO2 + RO2 reactions.	147.18

Table S-3

Variable Parameters in the SAPRC07TB Mechanism

Variable Parameter	Definition
RO2NO	K{BR07}*C{NO}
RO2HO2	K{BR08}*C{HO2}
RO2NO3	K{BR09}*C{NO3}
RO2RO2	K{BR10}*C{MEO2} + K{BR11}*C{RO2C} + K{BR11}*C{RO2XC}
RO2RO3	K{BR25}*C{MECO3} + K{BR25}*C{RCO3} + K{BR25}*C{BZCO3} + K{BR25}*C{MACO3}
RO2RO	RO2NO + RO2NO3 + RO2RO3 + 0.5*RO2RO2
RO2XRO	RO2HO2 + 0.5*RO2RO2
RO2RO2M	0.5*RO2RO2
RO22NN	RO2NO3 + RO2RO3 + 0.5*RO2RO2

Notes:

Variable Parameters are reaction rates computed at every chemistry time step.

K{***name***} equals the rate constant of the reaction ***name*** in the mechanism listing.

C{***XX***} equals the concentration of species ***XX***.

Parameters lower on the list are computed based on values of parameters higher on the list.

1
2

Table S-4

Photolysis Rates used in the SAPRC07TB mechanism

Rate	Source for cross-section and quantum yield	Temperature Correction	Number Density Correction
ACET-06	ACET-06: CH3-CO-CH3 + HV = Radical products. IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet P7. This datasheet updated: 19th December 2005. Website: http://www.iupac-kinetic.ch.cam.ac.uk/. IUPAC recommendations used for both absorption cross sections and quantum yield.	For cross-section and quantum yield	For quantum yield
ACRO-09	ACRO-09: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies Evaluation Number 15. JPL Publication 06-2. July 10, 2006.The quantum yields were derived using the pressure and wavelength-dependent expression given by IUPAC (2005) for MVK, with the total pressure adjusted so that the radical forming photolysis rates for the chamber experiments are the same as those that fit the chamber data. Adjusted pressure = 1.50 atm.		For quantum yield
AFG1	AFG1: Photolysis of lumped photoreactive aromatic unsaturated dicarbonyl product. Based on 31.6% BUTEDIAL and 68.4% 4OX2PEAL with QY(BUTEDIAL) = 0.723 and QY(4OX2PEAL) = 1.000, From h:\mech\saprc06\phf.xls, "AFG1" sheet and based on h:\mech\saprc06\aroprods.xls. NO Quantum Yield data. Set to one.		
BACL-07	BACL-07: CH3COCOCH3 + HV = 2 CH3CO. Absorption cross sections from Plum et al (1983) as used in SAPRC-99 mechanism. Quantum yields calculated using the IUPAC (2005)-recommended expression for the pressure and wavelength-dependence quantum yields for methyl glyoxal, but with the effective pressure adjusted so the photolysis rate, relative to that for NO2, under ambient conditions is consistent with that measured by Klotz et al (2000) in the Euphore outdoor chamber.	For quantum yield	For quantum yield
BALD-06	BALD-06 : Benzaldehyde absorption cross sections recommended by Calvert et al (2002) From Lang (1961-1971) in hexane solution NO Quantum Yield data. Set to one.		

Table S-4

Photolysis Rates used in the SAPRC07TB mechanism

Rate	Source for cross-section and quantum yield	Temperature Correction	Number Density Correction
C2CHO	C2CHO: C2CHO + HV = C2H5. + CHO. IUPAC (1997)		For quantum yield
CCHO_R	CCHO_R: CCHO + HV = CH3 + CHO. IUPAC (1997)		For quantum yield
CL2	CL2: CL2 + HV = 2 CL. FROM IUPAC EVALUATION (1996). RECOMMEND UNIT QUANTUM YIELD. NO Quantum Yield data. Set to one.	For cross-section	
CLACET	CLACET: Chloroacetone absorption cross sections. NO Quantum Yield data. Set to one.		
CLCCHO	CLCCHO: Chloroacetaldehyde absorption cross sections. NASA (2006) evaluation, NO Quantum Yield data. Set to one.		
CLNO-06	CLNO-06: CLNO absorption cross sections recommended by IUPAC (2005) . Wavelength where absorption goes to zero est'd by extrapolation. NO Quantum Yield data. Set to one.		
CLNO2	CLNO2: CLNO2 + HV = CL + NO2. FROM IUPAC EVALUATION (1996). RECOMMEND UNIT QUANTUM YIELD. NO Quantum Yield data. Set to one.		
CLONO	CLONO: CLONO + HV = CL + NO2. FROM IUPAC EVALUATION (1996). NO Quantum Yield data. Set to one.		
CLONO2-1	CLONO2-1: CLONO2 + hv = CLO. + NO2. CLONO2 absorption cross sections and quantum yields recommended by IUPAC (2005)	For cross-section	
CLONO2-2	CLONO2-2: CLONO2 + hv = CL. + NO3. CLONO2 absorption cross sections and quantum yields recommended by IUPAC (2005).	For cross-section	
COOH	COOH: CH3OOH + HV = PRODUCTS. IUPAC (1997). Also recommend unit quantum yields.		
GLY-07M	GLY-07M: HCOCHO + HV = HCHO + H2. Absorption cross sections from Volkamer, R., P. Spietz, J. Burrows, and U. Platt (2005): "High-resolution absorption cross sections of glyoxal in the UV-vis and IR spectral ranges," J. Photochem. Photobiol. A, 172 35-46. Quantum yields at wavelengths below 350 nm derived from those used		

Table S-4

Photolysis Rates used in the SAPRC07TB mechanism

Rate	Source for cross-section and quantum yield	Temperature Correction	Number Density Correction
	for the radical forming process assuming total quantum yields of 1. Quantum yields at higher wavelengths assumed to decline exponentially at a rate that gives a 13% formaldehyde yield relative to photodecomposition under the conditions of Plum et al (1983).		
GLY-07R	GLY-07R: HCOCHO + HV = HCO. + HCO. Absorption cross sections from Volkamer, R., P. Spietz, J. Burrows, and U. Platt (2005): "High-resolution absorption cross sections of glyoxal in the UV-vis and IR spectral ranges," J. Photochem. Photobiol. A, 17235-46. Quantum yields at wavelengths below 350 nm based on the data of Zhu et al (1996) which are consistent with the data of Langford and Moore (1984). Quantum yields at higher wavelengths assumed to decline expodentially with wavelength at a rate that gives a photolysis rate relative to NO2 consistent with the data of Klotz et al (2000).		
H2O2	H2O2:H2O2 + HV = 2 OH. IUPAC (1997) Recommended.	For cross-section	
HCHOM-06	HCHOM-06: HCHO + HV = H2 + CO. IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet P1. This datasheet updated: 16th May 2002. Website: http://www.iupac-kinetic.ch.cam.ac.uk/. IUPAC recommendations used for both absorption cross sections and quantum yield. Quantum yields for wl < 0.360 interpolated.	For cross-section and quantum yield	For quantum yield
HCHOR-06	HCHOR-06: HCHO + HV = HCO. + H. IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet P1. This datasheet updated: 16th May 2002. Website: http://www.iupac-kinetic.ch.cam.ac.uk/. IUPAC recommendations used for both absorption cross sections and quantum yield. Quantum yields for wl < 0.360 interpolated.	For cross-section	
HNO3	HNO3: HNO3 + HV = products. IUPAC (1997) Recommendation , NO Quantum Yield data. Set to one.	For cross-section	
HNO4-06	HNO4-06: HO2NO2 + HV = PRODUCTS. NASA	For cross-	

Table S-4

Photolysis Rates used in the SAPRC07TB mechanism

Rate	Source for cross-section and quantum yield	Temperature Correction	Number Density Correction
	(2006) NO Quantum Yield data. Set to one.	section	
HOCCHO	HOCCHO : Glycolahdehyde photolysis. IUPAC Data Sheet P5, May 2002. From PhotDat.xls		
HOCL-06	HOCL-06: HOCL absorption cross sections recommended by IUPAC (2005). NO Quantum Yield data. Set to one.		
HONO-06	HONO-06: HONO + HV = HO. + NO. NASA (2006) recommended absorption cross sections. No recommendation on quantum yield. IUPAC (2005) recommendation (Data Sheet PNOx1, July, 2001) recommends unit quantum yields. (IUPAC recommended absorption cross sections are low resolution, so NASA values HNO		
IC3ONO2	IC3ONO2: I-C3H7ONO2 + HV = PRODUCTS. IUPAC (1997). Recommend assuming unit quantum yields. This has stronger absorption than n-C3-ONO2 and lower nitrates, but chosen as representative of lumped higher nitrates. NO Quantum Yield data. Set to one.	For cross-section	
MACR-06	MACR-06: Methacrolein total photolysis. Absorption cross sections from IUPAC Subcommittee on Gas Kinetic Data Evaluation Website: http://www.iupac-kinetic.ch.cam.ac.uk/. The quantum yields were derived using the pressure and wavelength-dependent expression given by IUPAC (2005) for MVK, with the total pressure adjusted so that the radical forming photolysis rates for the chamber experiments are the same as those that fit the chamber data.		For quantum yield
MEK-06	MEK-06: MEK absorption cross sections IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet P8! This datasheet updated: 5th December 2005. Website: http://www.iupac-kinetic.ch.cam.ac.uk/. NO Quantum Yield data. Set to one.	For quantum yield	For quantum yield

Table S-4

Photolysis Rates used in the SAPRC07TB mechanism

Rate	Source for cross-section and quantum yield	Temperature Correction	Number Density Correction
MGLY-06	MGLY-06: CH3COCHO + HV = CH3CO. + HCO. IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet P6. This datasheet updated: 16th January 2003. Website: http://www.iupac-kinetic.ch.cam.ac.uk/. Quantum yield calculated from the expression given for 472 torr N2. This "pressure" adjustment was made so the calculated photolysis rates for solar conditions would agree with the data of Klotz et al (2000) for the Euphore outdoor chamber.	For quantum yield	For quantum yield
MVK-06	MVK-06: MVK total photolysis. ! IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet P10. Website: http://www.iupac-kinetic.ch.cam.ac.uk/ This datasheet updated: 9th August 2002. Decline in absorption cross sections with wavelength above 395 nm estimated by linear interpolation. Quantum yields for all photodecomposition processes. IUPAC recommends ~60% for propene formation, rest radical forming routes. Quantum yields calculated for 1 atm overpredicts photolysis rates for chamber experiments that gives best fits to data. Effective pressure increased to 5 atm to give overall quantum yields that are consistent with modeling chamber data.		For quantum yield
NO2-06	NO2-06 : NO2 + HV = NO + O. From NASA (2006). Absorption cross sections are averages for wavelength intervals given. Data aligned to smallest wavelength intervals for abs. coefs and qy's.	For cross-section	
NO2EX	NO2EX: NO2 + HV = NO2*.From NASA (2006), for 294 K. Absorption cross sections are averages for wavelength intervals given. Data aligned to smallest wavelength intervals for abs. coefs and qy's.	For cross-section	
NO3NO-06	NO3NO-06: NO3 + HV = NO + O2. From NASA (2006), Quantum yields for wavelengths above 640 nm estimated by linear extrapolation.	For cross-section and quantum yield	

Table S-4

Photolysis Rates used in the SAPRC07TB mechanism

Rate	Source for cross-section and quantum yield	Temperature Correction	Number Density Correction
NO3NO2-6	NO3NO2-6: NO3 + HV = NO2 + O. From NASA (2006), Quantum yields for wavelengths above 640 nm estimated by linear extrapolation.	For cross-section and quantum yield	
O3O1D-06	O3O1D-06: O3 + HV = O1D + O2. NASA (2006) abs. Coefs and IUPAC (2006) quantum yields. Absorption cross sections from NASA (2006). Quantum yields are from IUPAC (2006) recommendation, interpolated to the NASA (2006) absorption cross section wavelengths. NASA (2006) does not give useable recommendations for the absorption cross sections, except at <305 and >329 nm, where they are consistent with the IUPAC recommendations. Formation of O1D assumed not to occur at the high wavelength band.	For cross-section and quantum yield	
O3O3P-06	O3O3P-06: O3 + HV = O3P + O2. Absorption cross sections from NASA (2006). Quantum yields are derived from the O1D quantum yields in the low wavelength. Unit quantum yields assumed in high wavelength region. Absorption cross sections below 829 nm are extrapolated	For cross-section and quantum yield	
PAA	PAA: Peroxy acetic acid absorption cross sections. Orlando, J. J. and G. S. Tyndall (2003): "Gas phase UV absorption spectra for peracetic acid, and for acetic acid monomers and dimers," J. Photochem. Photobiol A, 157, 161-166. NO Quantum Yield data. Set to one.		
PAN	PAN: PAN + HV = #.6 {MECO3 + NO2} + #.4 {MEO2 + CO2 + NO3}.IUPAC Data Sheet P21.updated: 12/19/05. Reaction reflects recommended quantum yields at 308 nm. NO Quantum Yield data. Set to one.	For cross-section	

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Table S-5

SAPRC07TB Reactions forming Secondary Aerosol Material

name	reactants	products	rate expression
{44 }	OH + SO2 --->	HO2 + SULF + SULRXN	k< 44> is a falloff expression using: ko = 3.300E-31 * (T/300)**(-4.30) kinf = 1.600E-12 F = 0.60, n=1.00
{BE06}	ISOPRENE + OH --->	0.907*xHO2 +0.986*RO2C +0.093*RO2XC +0.093*zRNO3 +0.624*xHCHO +0.23*xMACR +0.32*xMVK +0.357*xIPRD + yR6OOH + ISOPRXN	k<287> = 2.540E-11 * exp(410.0/T)
{BT09}	APIN + OH --->	0.799*xHO2 +0.004*xRCO3 +1.042*RO2C +0.197*RO2XC +0.197*zRNO3 +0.002*xCO +0.022*xHCHO +0.776*xRCHO +0.034*xACETONE +0.02*xMGLY +0.023*xBACL + yR6OOH + TRPRXN	k<291> = 1.210E-11 * exp(436.0/T)
{BE12}	BENZENE + OH --->	0.570*HO2 +0.290*xHO2 +0.116*OH +0.29*RO2C +0.024*RO2XC +0.024*zRNO3 +0.29*xGLY +0.57*CRES +0.029*xAFG1 +0.261*xAFG2 +0.116*AFG3 +0.314*yRAOOH + BENZRO2	k<297> = 2.330E-12 * exp(-193.0/T)
{AE51}	BENZRO2 + NO --->	NO + BNZNRXN	k<402> = 1.000E+00 * k(56)
{AE52}	BENZRO2 + HO2 --->	HO2 + BNZHRXN	k<403> = 1.000E+00 * k(57)
{BT13}	TOLUENE + OH --->	0.181*HO2 +0.454*xHO2 +0.312*OH +0.454*RO2C +0.054*RO2XC +0.054*zRNO3 +0.238*xGLY +0.151*xMGLY +0.181*CRES +0.065*xBALD +0.195*xAFG1 +0.195*xAFG2 +0.312*AFG3 +0.073*yR6OOH +0.435*yRAOOH + TOLRO2	k<298> = 1.810E-12 * exp(338.0/T)
{BL14}	ARO1 + OH --->	0.123*HO2 +0.566*xHO2 +0.202*OH +0.566*RO2C +0.11*RO2XC +0.11*zRNO3 +0.158*xGLY +0.1*xMGLY +0.123*CRES +0.072*xAFG1 +0.185*xAFG2 +0.202*AFG3 +0.309*xPROD2 +0.369*yR6OOH + TOLRO2	k<317> = 7.840E-12

Table S-5

SAPRC07TB Reactions forming Secondary Aerosol Material

name	reactants	products	rate expression
{AE55}	TOLRO2 + NO --->	NO + TOLNRXN	k<406> = 1.000E+00 * k(56)
{AE56}	TOLRO2 + HO2 --->	HO2 + TOLHRXN	k<407> = 1.000E+00 * k(57)
{BT14}	MXYL + OH --->	0.159*HO2 +0.520*xHO2 +0.239*OH +0.52*RO2C +0.082*RO2XC +0.082*zRNO3 +0.1*xGLY +0.38*xMGLY +0.159*CRES +0.041*xBALD +0.336*xAFG1 +0.144*xAFG2 +0.239*AFG3 +0.047*yR6OOH +0.555*yRAOOH + XYLRO2	k<299> = 2.310E-11
{BT15}	OXYL + OH --->	0.161*HO2 +0.554*xHO2 +0.198*OH +0.554*RO2C +0.087*RO2XC +0.087*zRNO3 +0.084*xGLY +0.238*xMGLY +0.185*xBACL +0.161*CRES +0.047*xBALD +0.253*xAFG1 +0.253*xAFG2 +0.198*AFG3 +0.055*yR6OOH +0.586*yRAOOH + XYLRO2	k<300> = 1.360E-11
{BT16}	PXYL + OH --->	0.159*HO2 +0.487*xHO2 +0.278*OH +0.487*RO2C +0.076*RO2XC +0.076*zRNO3 +0.286*xGLY +0.112*xMGLY +0.159*CRES +0.088*xBALD +0.045*xAFG1 +0.067*xAFG2 +0.278*AFG3 +0.286*xAFG3 +0.102*yR6OOH +0.461*yRAOOH + XYLRO2	k<301> = 1.430E-11
{BT17}	TRIMETH_BENZ + OH --->	0.022*HO2 +0.627*xHO2 +0.230*OH +0.627*RO2C +0.121*RO2XC +0.121*zRNO3 +0.074*xGLY +0.405*xMGLY +0.112*xBACL +0.022*CRES +0.036*xBALD +0.088*xAFG1 +0.352*xAFG2 +0.23*AFG3 +0.151*xAFG3 +0.043*yR6OOH +0.705*yRAOOH + XYLRO2	k<302> = 3.250E-11
{BL15}	ARO2 + OH --->	0.077*HO2 +0.617*xHO2 +0.178*OH +0.617*RO2C +0.128*RO2XC +0.128*zRNO3 +0.088*xGLY +0.312*xMGLY +0.134*xBACL +0.077*CRES +0.026*xBALD	k<318> = 3.090E-11

Table S-5

SAPRC07TB Reactions forming Secondary Aerosol Material

name	reactants	products	rate expression
		+0.221*xAFG1 +0.247*xAFG2 +0.178*AFG3 +0.068*xAFG3 +0.057*xPROD2 +0.101*yR6OOH + XYLRO2	
{AE53}	XYLRO2 + NO --->	NO + XYLNRXN	k<404> = 1.000E+00 * k(56)
{AE54}	XYLRO2 + HO2 --->	HO2 + XYLHRXN	k<405> = 1.000E+00 * k(57)
{BL05}	ALK5 + OH --->	0.647*xHO2 +1.605*RO2C +0.353*RO2XC +0.353*zRNO3 +0.04*xHCHO +0.106*xCCHO +0.209*xRCHO +0.071*xACETONE +0.086*xMEK +0.407*xPROD2 + yR6OOH + ALK5RXN	k<308> = 2.700E-12 * exp(374.0/T)
{BT11}	APIN + NO3 --->	0.056*xHO2 +0.643*xNO2 +0.007*xRCO3 +1.05*RO2C +0.293*RO2XC +0.293*zRNO3 +0.005*xCO +0.007*xHCHO +0.684*xRCHO +0.069*xACETONE +0.002*xMGLY +0.056*xRNO3 + yR6OOH + TRPRXN	k<293> = 1.190E-12 * exp(490.0/T)
{BT12}	APIN + O3P --->	PRD2 + TRPRXN	k<294> = 3.200E-11
{BL16}	TERP + OH --->	0.734*xHO2 +0.064*xRCO3 +1.211*RO2C +0.201*RO2XC +0.201*zRNO3 +0.001*xCO +0.411*xHCHO +0.385*xRCHO +0.037*xACETONE +0.007*xMEK +0.003*xMGLY +0.009*xBACL +0.003*xMVK +0.002*xIPRD +0.409*xPROD2 + yR6OOH + TRPRXN	k<319> = 2.270E-11 * exp(435.0/T)
{BL18}	TERP + NO3 --->	0.227*xHO2 +0.287*xNO2 +0.026*xRCO3 +1.786*RO2C +0.46*RO2XC +0.46*zRNO3 +0.012*xCO +0.023*xHCHO +0.002*xHOCCHO +0.403*xRCHO +0.239*xACETONE +0.005*xMACR +0.001*xMVK +0.004*xIPRD +0.228*xRNO3 + yR6OOH + TRPRXN	k<321> = 1.330E-12 * exp(490.0/T)
{BL19}	TERP + O3P --->	0.237*RCHO +0.763*PRD2 + TRPRXN	k<322> = 4.020E-11
{BT19}	SESQ + OH --->	0.734*xHO2 +0.064*xRCO3 +1.211*RO2C +0.201*RO2XC +0.201*zRNO3 +0.001*xCO	k<323> = 1.000E+00 * k(319)

Table S-5

SAPRC07TB Reactions forming Secondary Aerosol Material

name	reactants	products	rate expression
		+0.411*xHCHO +0.385*xRCHO +0.037*xACETONE +0.007*xMEK +0.003*xMGLY +0.009*xBACL +0.003*xMVK +0.002*xIPRD +0.409*xPROD2 + yR6OOH + SESQRXN	
{BT21}	SESQ + NO3 --->	0.227*xHO2 +0.287*xNO2 +0.026*xRCO3 +1.786*RO2C +0.46*RO2XC +0.46*zRNO3 +0.012*xCO +0.023*xHCHO +0.002*xCCHO +0.403*xRCHO +0.239*xACETONE +0.005*xMACR +0.001*xMVK +0.004*xIPRD +0.228*xRNO3 + yR6OOH + SESQRXN	k<325> = 1.000E+00 * k(321)
{BT22}	SESQ + O3P --->	0.237*RCHO +0.763*PRD2 + SESQRXN	k<326> = 1.000E+00 * k(322)

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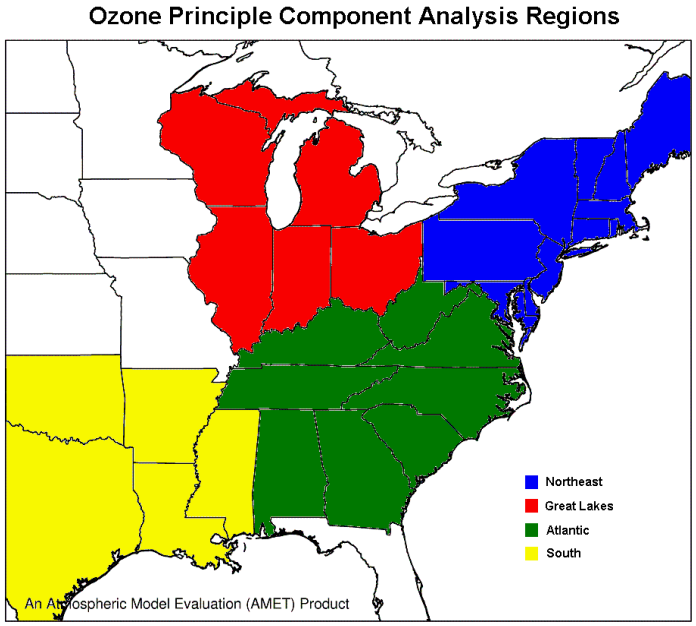


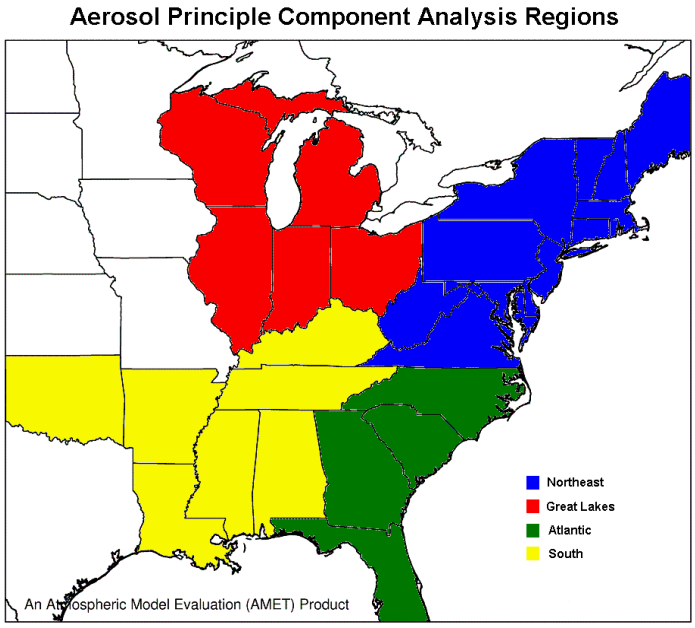


Figure S-1: States comprising the PCA regions for the ozone and aerosol regional analyses

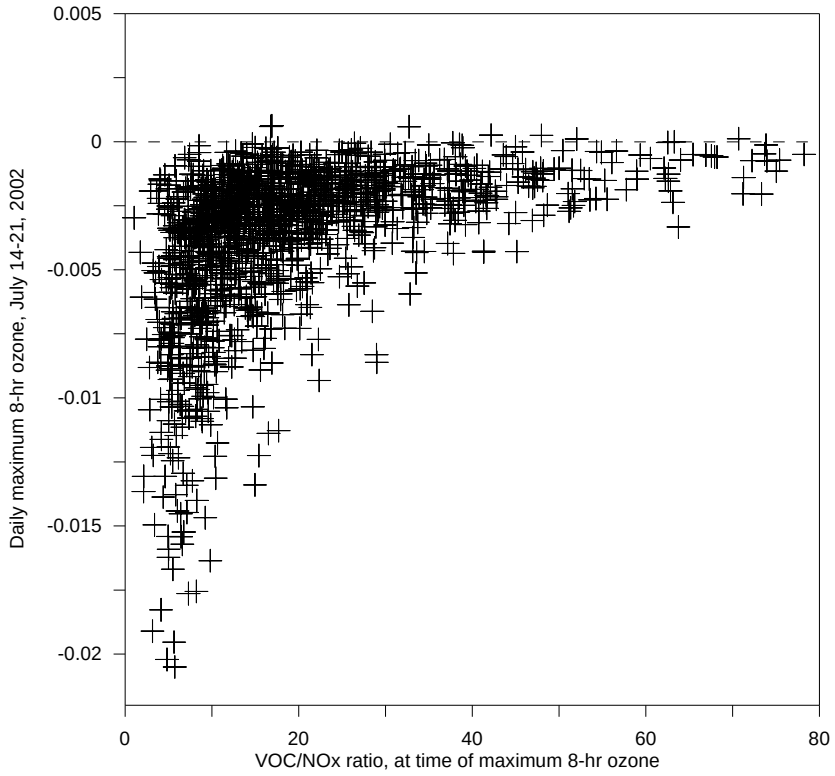


Figure S-2: The scatter plot shows SAPRC07T minus SAPRC-99 in daily maximums in the 8-hr averages for ozone over the Great Lakes region as a function of the 8-hour VOC/NOx ratio, from July 14 to 21, 2002.

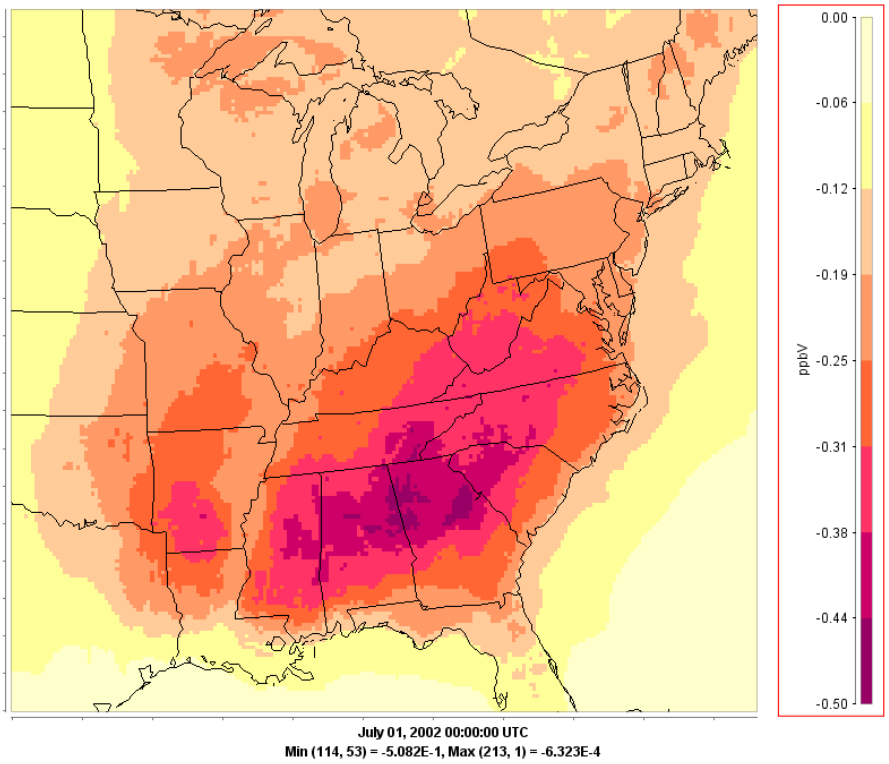


Figure S-3: SAPRC07T minus SAPRC-99 is shown for total PAN averaged over July.

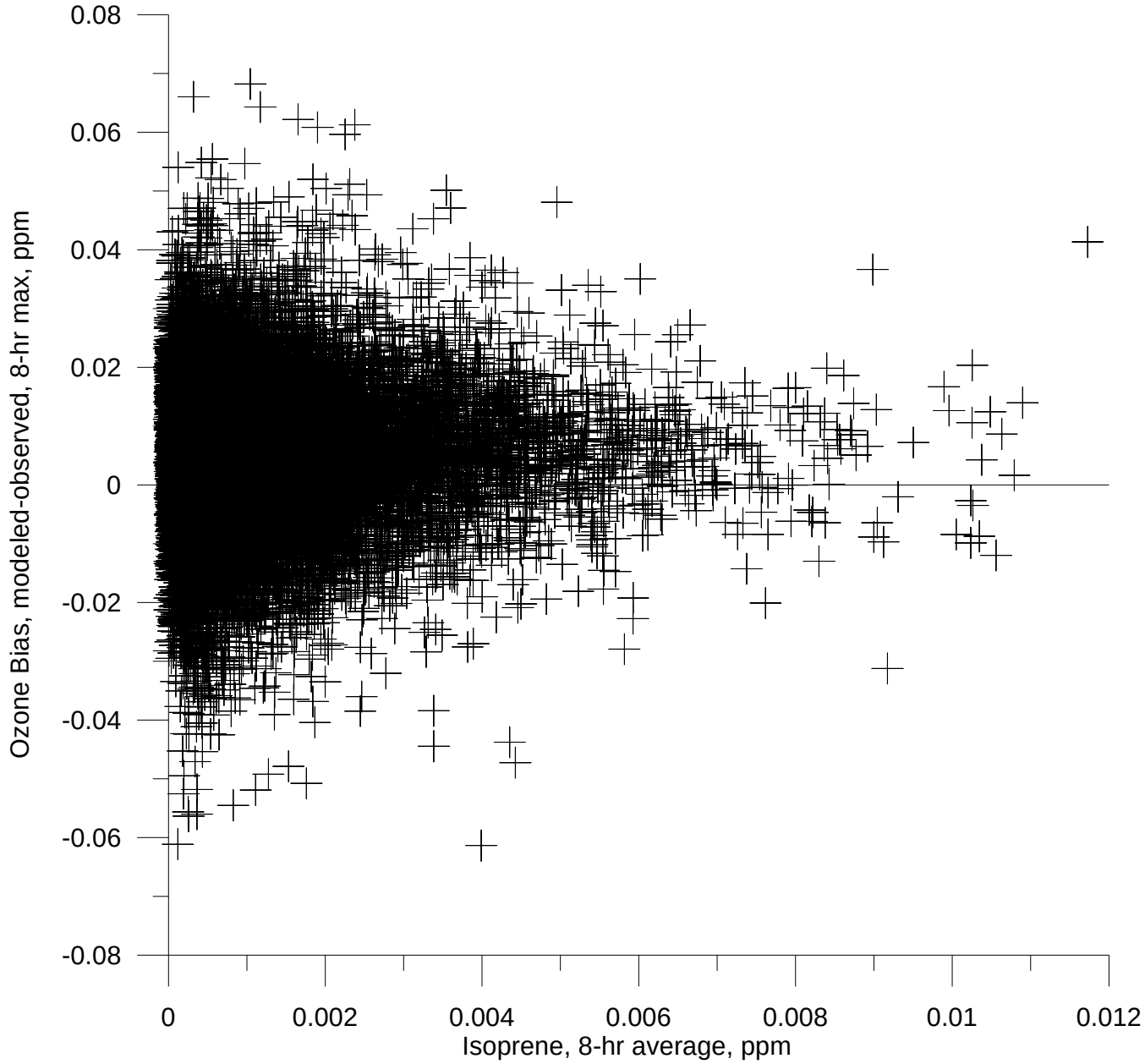
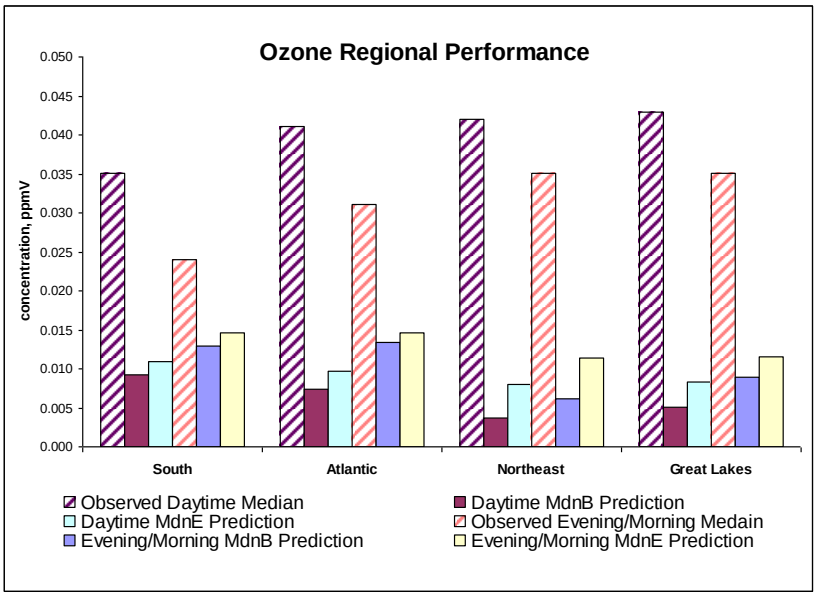


Figure S-4: O3 bias as a function of modeled ISOPRENE.



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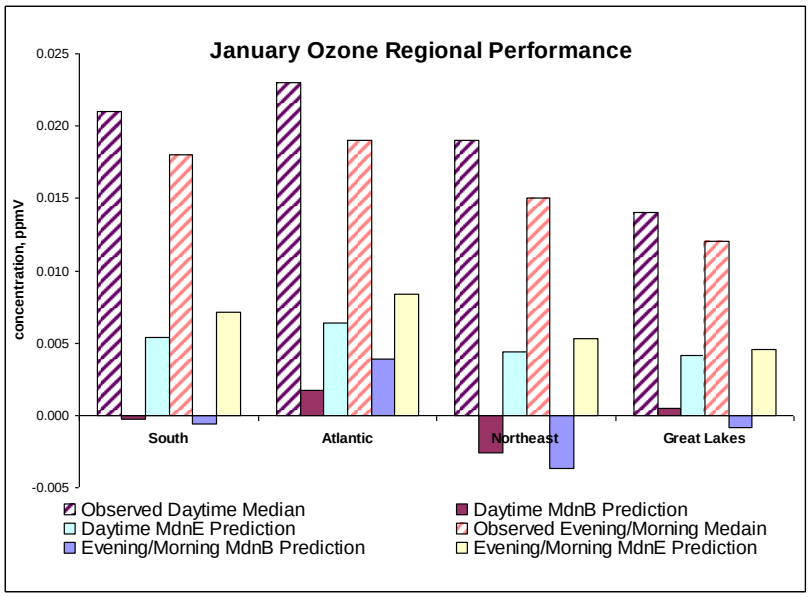


2
3

4 Figure S-5. Observed ozone and SAPRC07T median bias and error during July (Top) and
5 January (Bottom) 2002 in terms of the Median Error (MdnE) and Median Bias (MdnB). The
6 measures are given as a function of geographical region and time of the day. Daytime results
7 represent observations between 7 am to 4 pm local standard time. Evening/morning results
8 represent observations from the remaining hours.
9

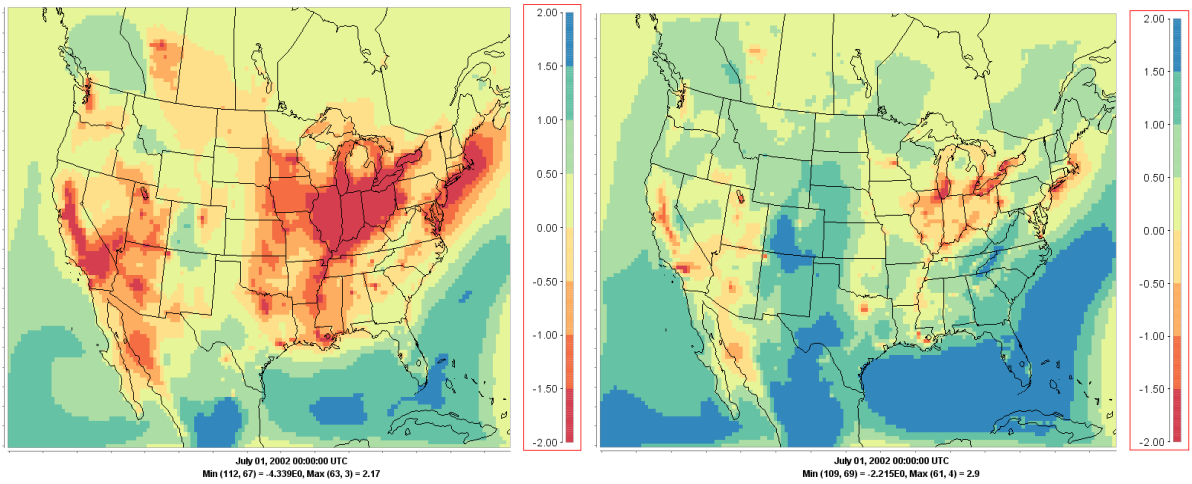
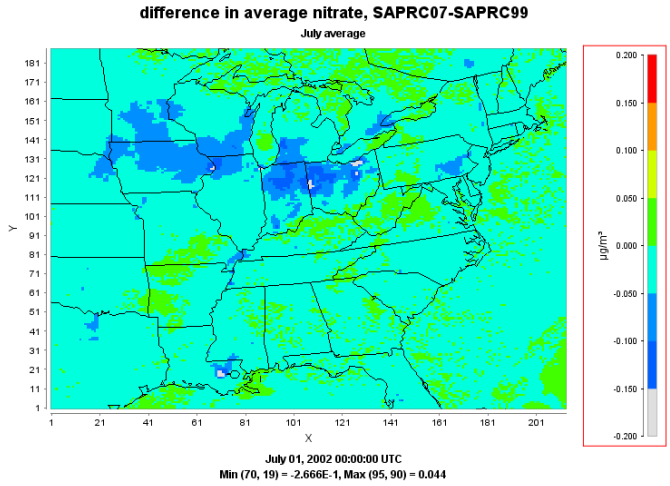
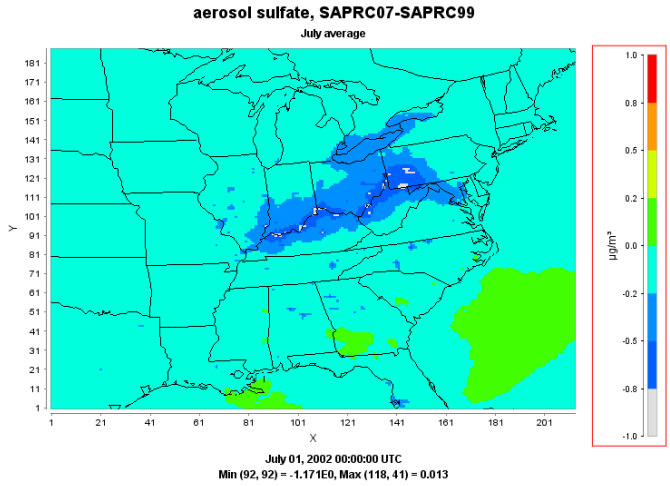


Figure S-6: Difference in average ozone between SAPRC07T minus SAPRC-99 (left) and between SAPRC07T with lowered OH+NO2 reaction rate minus SAPRC-99 (right). Units are ppb.





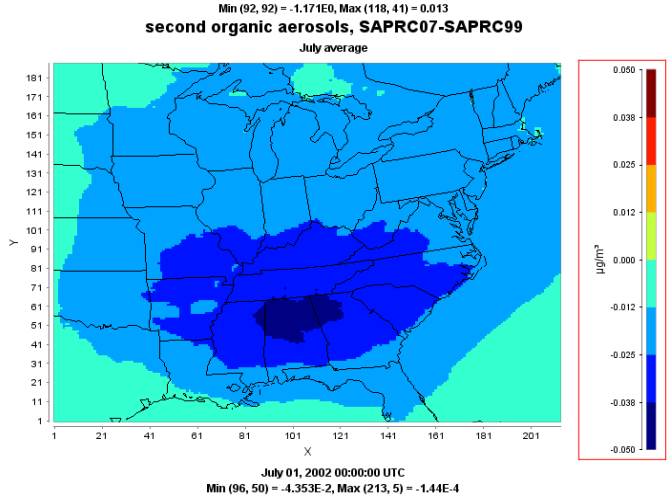


Figure S-7: SAPRC07 minus SAPRC-99 are shown for nitrate (top), sulfate (middle), secondary organic aerosols (bottom) in $PM_{2.5}$.