Supporting Information

Examining the Temperature Dependence of E85 Versus Gasoline Emissions on Air Pollution with a Near-Explicit Chemical Mechanism

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Summary
The supporting information document includes 1) a detailed description of the model used for this study, 2) more details about the speed and accuracy validation of the model, 3) additional model setup information including the tables of emissions, 4) discussion of the time-series results not included in the main paper, and 5) more sensitivity results.

1. Model Description

This air pollution box model combines a near-explicit chemical mechanism with a sparse-matrix ordinary differential equation solver.

1A. Chemical Mechanism

Master Chemical Mechanism version 3.1 (MCM)

The Master Chemical Mechanism (MCM) version 3.1 was chosen for this study because it is a near-explicit chemical mechanism that has been evaluated previously. MCM v. 3.1 (updated 2005) describes the tropospheric degradation of 135 commonly-emitted volatile organic compounds (VOCs) (Jenkin et al. 1997; MCM 2002; Jenkin et al. 2003; Saunders et al. 2003; Bloss et al. 2005b). It currently incorporates over 13,500 chemical reactions and over 4,600 species.

A number of studies have looked at the accuracy of the MCM v. 3 and v. 3.1 by comparing the model results with smog chamber data, including for the species examined here (Wagner et al. 2002; Bloss et al. 2005a; Bloss et al. 2005b; Hynes et al. 2005; Pinho et al. 2005; Pinho et al. 2006a; Pinho et al. 2006b; Pinho et al. 2007). The mechanism has also been used in a number of field studies, often in conjunction with a photochemical trajectory model (PTM), to assess ozone formation in the atmosphere (Derwent et al. 2003; Derwent et al. 2005; Derwent et al. 2007; Evtyugina et al. 2007) and to look at secondary organic aerosol formation (Jenkin 2004; Johnson et al. 2004; 2005; Johnson et al. 2006a; Johnson et al. 2006b). The uncertainties associated with the MCM have also been investigated (Zador et al. 2005).

1B. Ordinary Differential Equation Solver

Sparse-Matrix Vectorized Gear Solver (SMVGEAR II)

To solve the large set of chemical equations in the MCM, we use SMVGEAR II, a sparse-matrix ordinary differential equation (ODE) solver (Jacobson and Turco 1994; Jacobson 1995; 1998). It was chosen for several reasons. First, it uses the Gear solution mechanism, which is considered a benchmark for accuracy. Second, it uses a sparse-matrix technique during matrix decomposition and backsubstitution that dramatically decreases the run times. Jacobson (1995; 1998) also describes other measures that SMVGEAR employs to decrease run time for 3D modeling, including grouping and reordering of cells. The speed of the ODE solver is very important for allowing a large mechanism such as MCM to be used in urban, regional, and global 3-D models.

2. Mechanism Evaluation

Here, the accuracy of the MCM 3.1 against smog chamber data and the speed of its solution within SMVGEAR II are evaluated. The near-explicit MCM is also compared with a condensed mechanism, using the same ODE solver, SMVGEAR II, to model both mechanisms. Since condensed mechanisms are widely used, for example by air pollution control agencies to predict air pollution changes with particular reductions in emissions, it is important to see how the near-explicit MCM matches up to a condensed mechanism. An Adjusted Carbon Bond Mechanism (ACBM) was chosen for the condensed mechanism.

2A. Adjusted Carbon Bond Mechanism (ACBM)

The Adjusted Carbon Bond Mechanism (ACBM) used here (Jacobson 2007b) has 188 species, 374 kinetic reactions (with 51 inorganic reactions) and 66 photolysis reactions. It is based on the Expanded Carbon Bond IV (CBIV) mechanism (Gery et al. 1989) with updates to the inorganic reactions and some additional explicit treatment. Although most species are lumped, some are treated explicitly for their initial degradation, like toluene and propene. Their intermediate species, though, are still lumped. A complete listing of the reactions in the ACBM can be found in the supplementary information in Jacobson (2007b).

2B. Model Speed Validation

As discussed in the main text, SMVGEAR II dramatically reduces the number of multiplications required to perform decomposition and backsubstitution to solve large chemical mechanisms like the MCM (main text Table 1). Here we compared an older version of the ACBM that had 140 species and 277 reactions, MCM v. 2.0 with 2325 species and 6965 reactions, and the MCM v. 3.1 with 4649 species and 13566 reactions. Liang and Jacobson (2000) previously looked at the speed of SMVGEAR II with a smaller ACBM (109 species, 233 reactions) (Jacobson 1999) and MCM v. 1.0 (1427 species and 3911 reactions) (Jenkin et al. 1997). Their data plus our data shows how the efficiency increases as the number of species increases, as shown in Figure S1. Figure S2 shows the computer run time for a box model and for 450 grid cells on an Intel Pentium 4 Extreme, a 3.2 GHz machine for three chemical mechanism sizes, the older ACBM, MCM v.2.0, and MCM v. 3.1. The model took one minute to run 24 hours with MCM v. 3.1 (the 4649-species case) in box mode. In 450 cells, the run time was about 4 minutes or 113 times faster per cell than in one cell. This increasing efficiency with an increase in the number of grid cells was due to the vectorization technique in SMVGEAR II, which also reduces computer time on scalar machines (Jacobson 1998). The time is also much less than the approximately 220 days without the sparse-matrix technique. Only 8.1 times more computer time is needed for MCM v. 3.1 instead of the older ACBM, even though the number of species increases by 33 times and the number of reactions increases by 49 times. This sparse-matrix reduction makes it very reasonable to run large chemistry sets like MCM in a 3-D local, regional, or global model, as was demonstrated in a recent study by Jacobson and Ginnebaugh (~~2009~~). The authors show that only ~3.7 times more overall computer time for all model processes was necessary when increasing the number of species and reactions by 31 and 46 times, respectively, in a 3-D global-through-urban climate-weather-air pollution model.

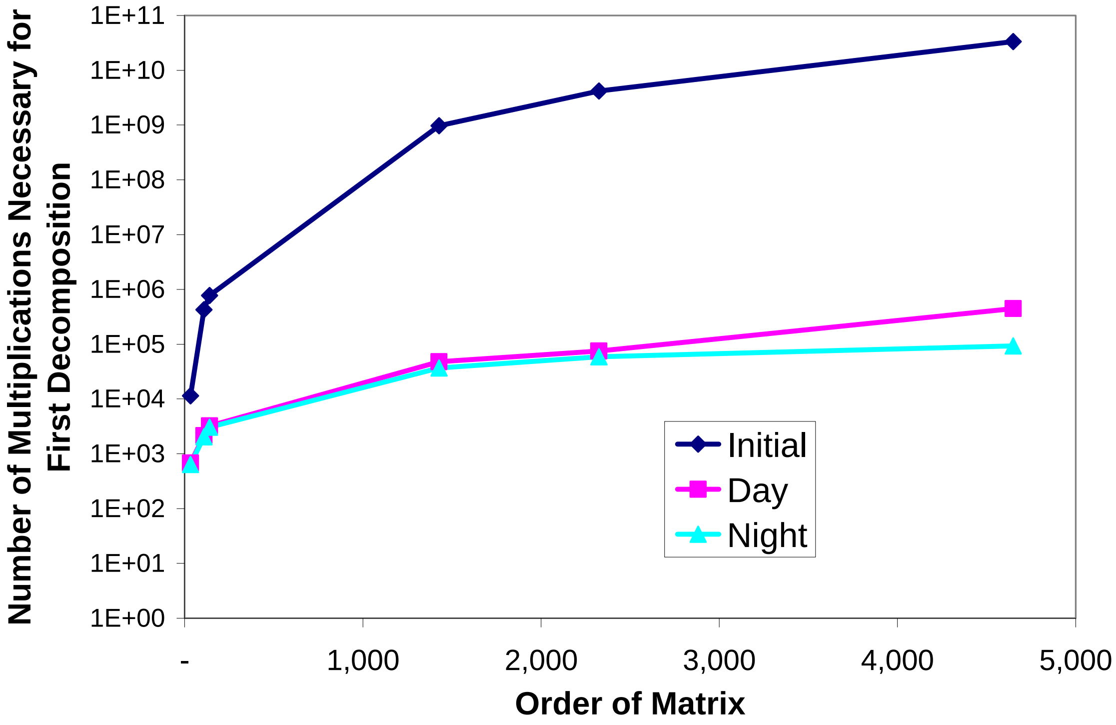

Figure S1: SMVGEAR II Reductions in Number of Multiplications Required in First Loop of Matrix Decomposition versus Order of Matrix between when No Sparse Matrix Techniques are Used ("Initial") and when Sparse Matrix Techniques are Used During Day and Night Chemistry ("Day", "Night")

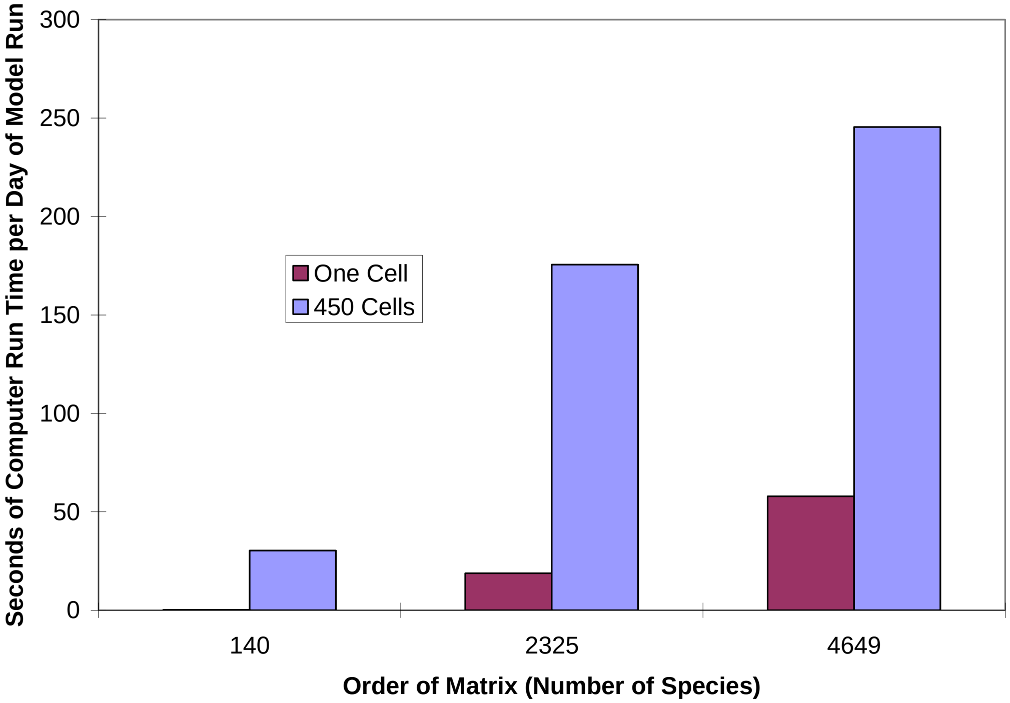

Figure S2: Computer Timings for 24 hrs of Model Time with SMVGEAR II for older ACBM (140 species), MCM v. 2 (2325 species) and MCM v. 3.1 (4649 species). Note: These numbers do not include the initialization time, which may be significant for short (12 hr – 24 hr) runs but would only be a small portion of the total run time for longer runs.

2C. MCM versus Smog Chamber Data

To test the accuracy of MCM v. 3.1, we compare it with smog chamber data. The current ACBM was also compared with data. Here, we compare the results for four species: two alkenes (propene and 1-butene) and two aromatics (toluene and m-xylene). The initial conditions for each scenario are shown in Table S1.

Smog Chamber Conditions for Each Case

	Species	Initial (ppbv)	Final (ppbv)
Indoor Smog Chamber			
1-Butene Case	1-Butene	315	
	NO	96	
	H_2O (25% RH)	1,200,000	
	Temperature (K)	297.2	
Propene Case	Propene	335	
	NO	96	
	CO	200	
	H_2O (25% RH)	7,008,630	
	Temperature (K)	296.4	
Outdoor Smog Chamber			
Toluene Case	Toluene	702	
JN2784B	C_2H_4	122	
	NO	300	
	NO_2	35	
	HONO	2.45	
	CO	300	
	H_2O	20,000,000	38,000,000
	Temperature (K)	293.8	311.8
m-Xylene case	m-Xylene	249	
JN2784R	NO	303	
	NO_2	40	
	HONO	1	
	CO	213	
	HCHO	10	
	H_2O	20,000,000	38,000,000
	Temperature (K)	293.8	311.8

Table S1: Smog Chamber Initial and Final Conditions for the Indoor and Outdoor Smog Chambers

Indoor Smog Chamber

The two alkenes, propene and 1-butene, were investigated using indoor smog chamber data from Australia's Commonwealth Scientific and Industrial Research Organization (CSIRO) laboratories (Hynes et al. 2005). The chamber used a UV lamp instead of sunlight to initiate photolysis, so the light intensity in the model was kept constant throughout the experiment. The UV lamp did not represent the full range of wavelengths from sunlight, so the photolysis rates in MCM had to be adjusted accordingly (Hynes et al. 2005). These rates were based on measured nitrogen dioxide (NO_2) photolysis rates and were provided by the authors.

Other adjustments to the model included the addition of wall reactions (Table S2) and reactions for the degradation of the organic species by atomic oxygen, $O(^3P)$, which have been found to be important in a confined area like a smog chamber (Table S3) (Carter 2000).

Wall Reactions for Indoor Smog Chamber			
Reaction	**Reaction Rate**	**Range**	**Notes**
hv + wall -> OH	4.89×10^{5}	J_{NO2} (0.00075-0.0030) ppbv s^{-1}	wall was treated as a species with a constant mixing ratio of 4.09×10^{-20}
hv + wall -> NO_2	4.89×10^{5}	J_{NO2} (0.00075-0.0030) ppbv s^{-1}	
NO_2 -> 0.5 HONO + 0.5 wall-HNO_3	1×10^{-6} s^{-1}	5×10^{-7} - 2×10^{-6} s^{-1}	
N_2O_5 -> 2 wall-HNO_3	1×10^{-5} s^{-1}	5×10^{-7} - 2×10^{-6} s^{-1}	
N_2O_5 + H_2O -> 2 wall-HNO_3	1×10^{-20} cm^3 s^{-1}	1×10^{-21} - 1×10^{-19} cm^3 s^{-1}	
Wall-HNO_3 + *hv* -> OH + NO_2	6.41×10^{-8} s^{-1}	(0.5 - 2.0) J_{HNO3}	
HNO_3 -> wall-HNO_3	1×10^{-4} s^{-1}	5×10^{-5} - 2×10^{-4} s^{-1}	
NO_2 -> wall	2×10^{-7} s^{-1}	1×10^{-7} - 4×10^{-7} s^{-1}	
O_3 -> wall	2×10^{-7} s^{-1}	1×10^{-7} - 4×10^{-7} s^{-1}	

Table S2: Wall Reactions from the Teflon Walls of the Indoor Smog Chamber

Note: Measured and Provided by Hynes et al. (2005)

Additional Reactions for Degradation by $O(^3P)$ in Indoor Smog Chamber		
	Reaction	**Reaction Rate**
Propene	$C_3H_6 + O(^3P)$ -> C_3H_6O	4×10^{-12} cm^3 s^{-1}
	$C_3H_6 + O(^3P)$ -> C_2H_5CHO	4×10^{-12} cm^3 s^{-1}
	$C_3H_6 + O(^3P)$ $(+2O_2)$ -> $HC(O)CH_2O_2 + CH_3O_2$	4×10^{-12} cm^3 s^{-1}
	$C_3H_6 + O(^3P)$ $(+2O_2)$ -> $C_2H_5O_2 + HO_2 + CO$	4×10^{-12} cm^3 s^{-1}
	$C_3H_6O + OH$ $(+O_2)$ -> $CH_3C(O)CH_2O_2$	8×10^{-13} cm^3 s^{-1}
1-Butene	1-$C_4H_8 + O(^3P)$ -> C_4H_8O	1.83×10^{-12} cm^3 s^{-1}
	1-$C_4H_8 + O(^3P)$ -> C_3H_7CHO	1.62×10^{-12} cm^3 s^{-1}
	1-$C_4H_8 + O(^3P)$ $(+2O_2)$ -> $HC(O)CH_2O_2 + C_2H_5O_2$	7.06×10^{-13} cm^3 s^{-1}
	$C_4H_8O + OH$ $(+O_2)$ -> $CH_3CH_2C(O)CH_2O_2$	1×10^{-12} cm^3 s^{-1}

Table S3: Additional Reactions Added to the Mechanism for the Indoor Smog Chamber Cases, 1-Butene and Propene

Note: Reactions Provided by Hynes et al. (2005)

The temperature of the smog chamber increased throughout the experiment from the UV lamp so the model had to be modified accordingly (Figure S3). The temperature increased by 6 K in the first 15 minutes, then by 5 K over the next 5.5 hours. The increase was assumed to be linear. The profile was the same for the propene and the 1-butene cases, except that their starting temperatures were 296.4 K and 297.2 K, respectively.

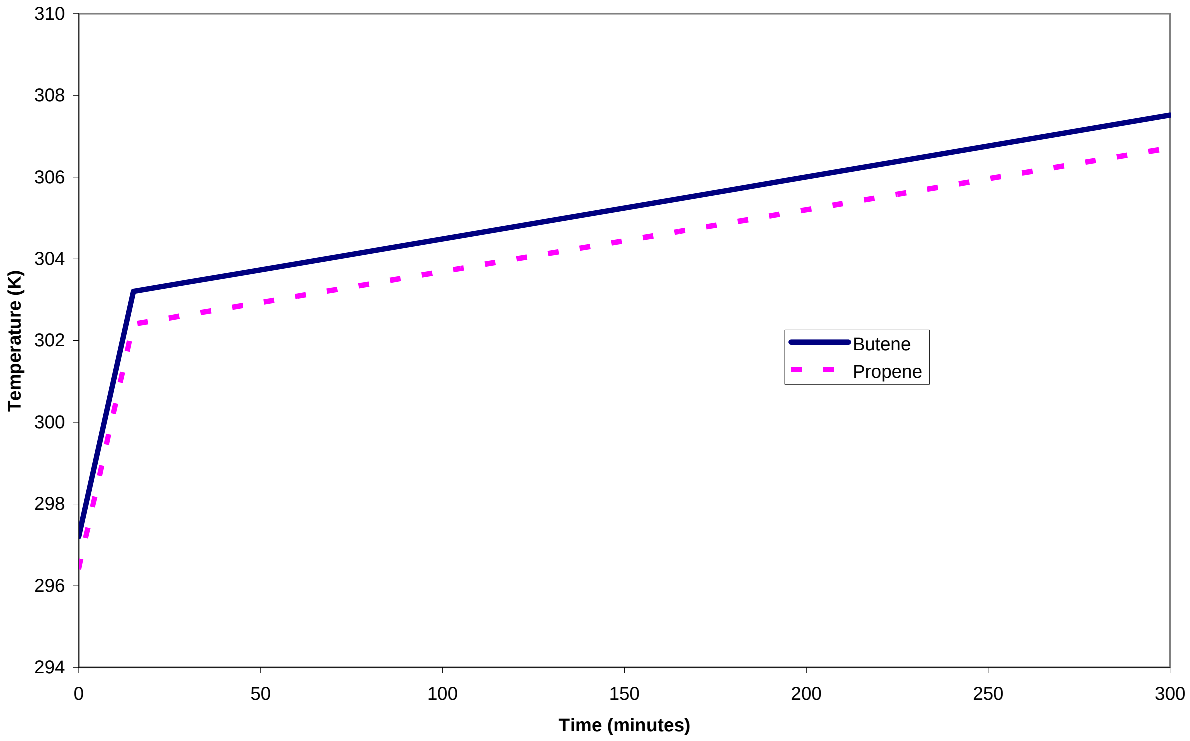

Figure S3: Temperature Profile for Indoor Smog Chamber for 1-Butene and Propene Cases

The model also had to be adjusted to account for dilution. The air inside a smog chamber is often diluted with ambient air when the sampling system draws air out of the chamber to be analyzed. The reaction rates are impacted by the reduced species concentration. The dilution rates used were 10.5 L/min for the propene case and 20 L/min for the 1-butene case (Hynes et al. 2005).

Sensitivity to Wall Reactions

Wall reactions produce the hydroxyl radical (OH) and NO_2 and affix nitric acid (HNO_3), NO_2, and ozone (O_3) to the smog-chamber wall. The high and low reaction rates for each wall reaction (Hynes et al. 2005), shown in Table S2, were modeled for the propene case to determine the sensitivity of the results to the wall reactions. The impact was minimal except for nitrogen pentoxide (N_2O_5) combining with water (H_2O) to form nitric acid affixed to the wall ($N_2O_5 + H_2O \rightarrow$ Wall-HNO_3), where the peak ozone differed by 37 ppb when using the high versus the low reaction rate. This may be because the range for the reaction rate of this wall reaction was relatively large. There was not much change in ozone when using the high or low values for the other reactions. Therefore, the middle of the range was used for the 1-butene and propene model predictions.

Sensitivity to Temperature

The model results were sensitive to the temperature profile used (not shown). Tests were performed for the propene case with different temperature profiles, such as an average temperature, a linear increase, and the profile shown in Figure S3**.** The model predictions did not accurately predict the data in either magnitude or the timing of peaks until the temperature profile was modified to match the indoor chamber conditions. Temperature proved to be a very important factor in accurately modeling the data.

Sensitivity to Dilution

To examine the sensitivity of the results to the dilution rates, the scenarios were modeled for full dilution rates (10.5 L/min for propene, 20 L/min for 1-butene), half dilution rates (5.25 L/min for propene, 10 L/min for 1-butene) and no dilution, at a 15 minute time step. They were also modeled for a smaller time step, 3 minutes and 45 seconds, but the smaller time step did not change the results. The results for different dilution rates for 15 minute time steps are shown in Figure S4 for a few species.

The dilution rate had a significant impact on model predictions. The difference between no dilution and full dilution was larger for species with larger concentrations. The difference also increased as the species concentration increased, and decreased with decreasing concentration. For example, peak ozone was 108.5 ppb (30%) higher for the no dilution case than for the full dilution case in the 1-butene scenario. For the propene scenario, the no dilution ozone peak was 81.6 ppb (16%) higher than the ozone peak for the full dilution case. Dilution caused a significant reduction in the modeled peak of ozone for both 1-butene and propene. The full dilution case was used in for the final model comparison because this most accurately represents the smog chamber conditions.

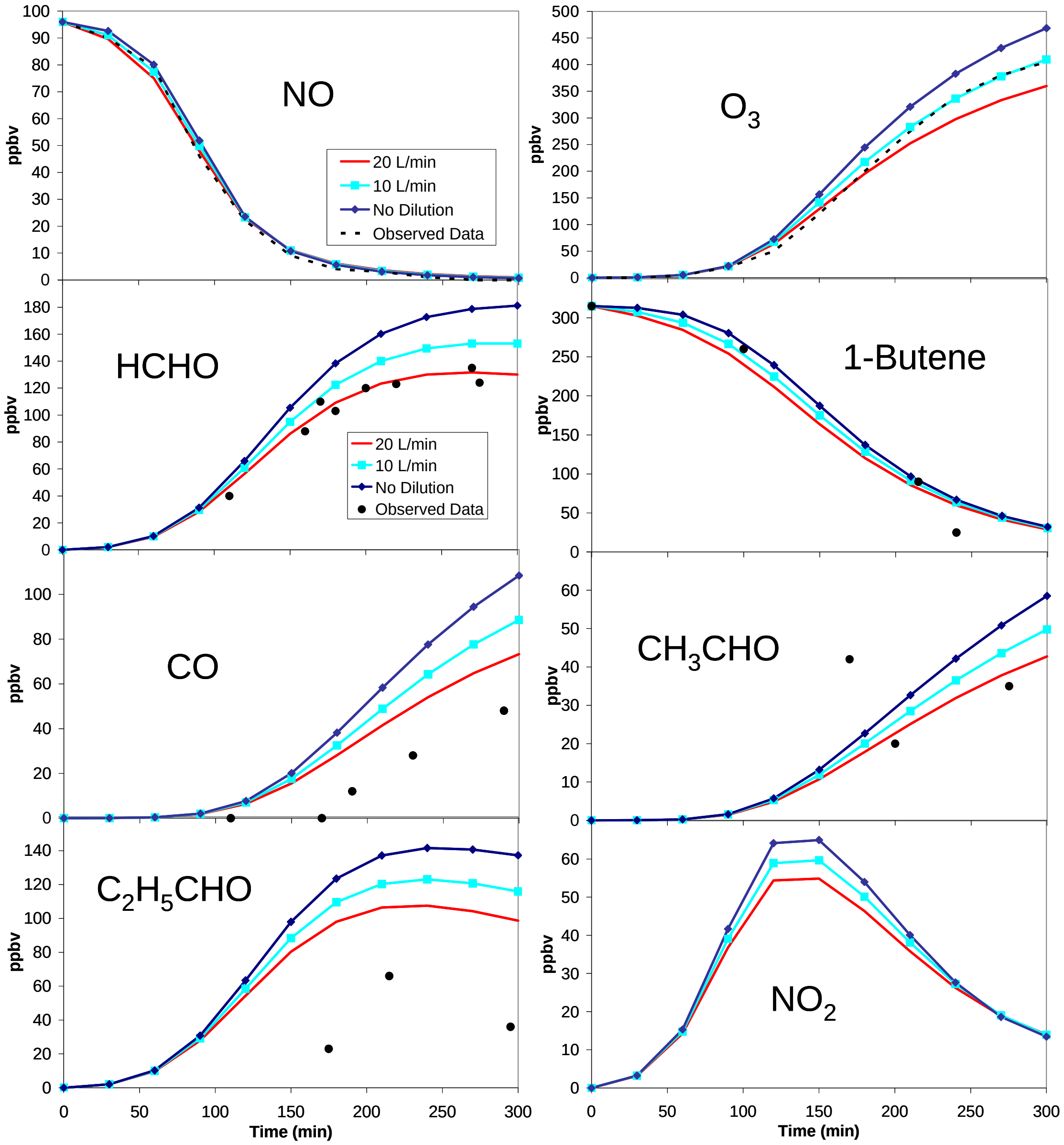

Figure S4: Dilution Model Comparison for the 1-Butene Case

Note: Observed Data is from Hynes et al. (2005)

1-Butene Case

The ACBM does not treat 1-butene explicitly so it was not compared to the MCM for this case. The MCM model predictions for the 1-butene case for nitric oxide (NO), formaldehyde (HCHO), acetaldehyde (CH_3CHO), and 1-butene (1-C_4H_8) followed the observed data (Hynes et al. 2005) closely, although the data for 1-butene and acetaldehyde were sparse (Figure S5). The MCM model captured 89% of the peak for ozone (O_3), under-predicting it by 45 parts-per-billion volume (ppbv). The timing of the increase in ozone concentration was good. The MCM model over-predicted the formation of propanal (C_2H_5CHO) and carbon monoxide (CO) but it did appear to get the shape of the trends correct. The over-prediction of the formation of propanal was difficult to quantify because the peak amount may not have been captured in the few data points. For carbon monoxide, the modeled peak was a factor of 1.5 higher than were the measurements. Nitrogen dioxide (NO_2) showed the typical peak and decline in concentration, but the data was only presented as NO_y and therefore not available for this comparison.

Propene Case

The propene case is discussed in the main text.

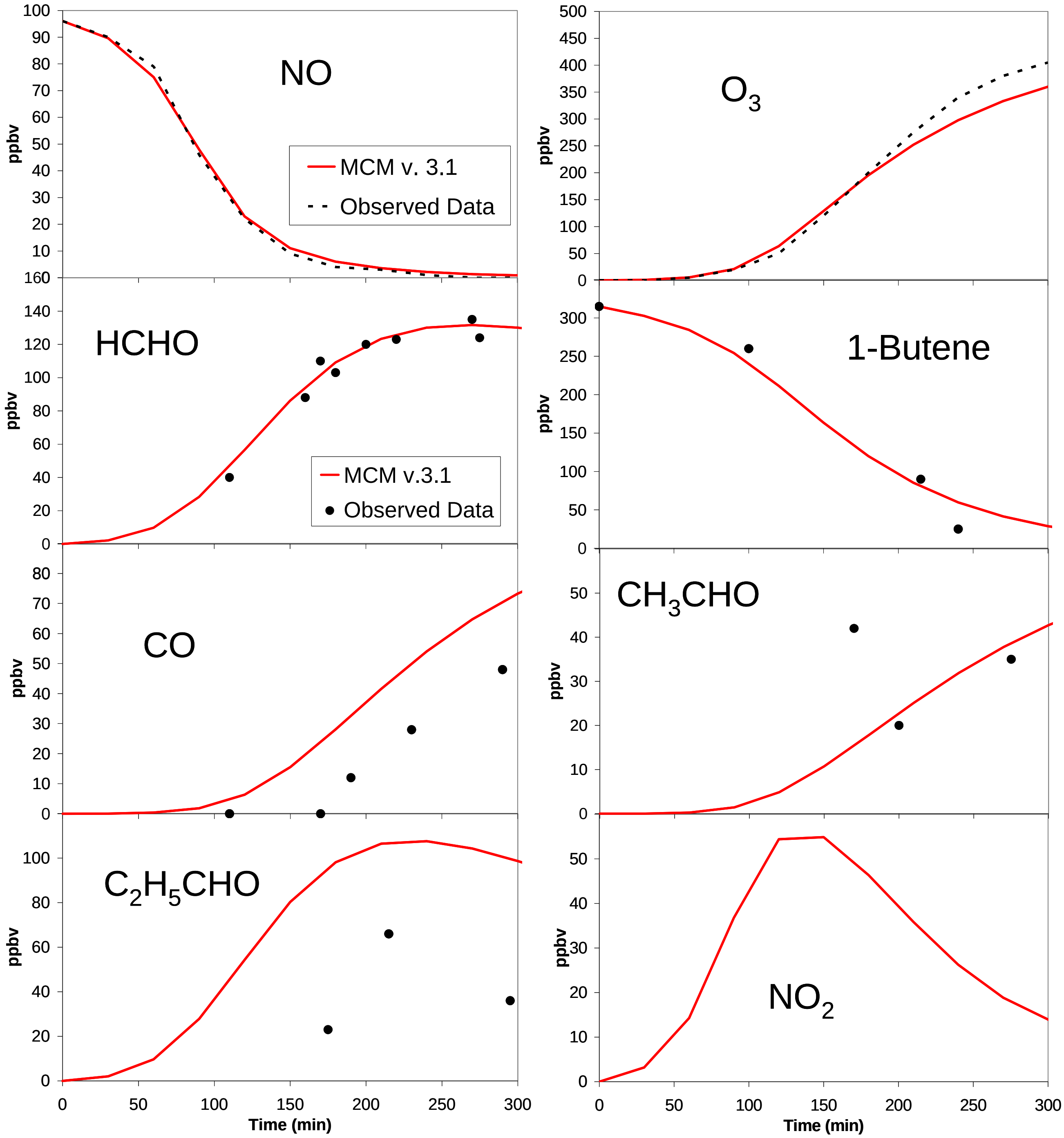

Figure S5: Observed and Modeled Results for 1-Butene Case using the Master Chemical Mechanism (MCM 3.1)

Note: Observed data from Hynes et al. (2005)

Outdoor Smog Chamber

The toluene and m-xylene data sets were from the University of North Carolina's large outdoor smog chamber (Gery et al. 1988). Both experiments were run on the same day, June 27, 1984, in the two separate halves of the chamber. These data sets were chosen because the light conditions were good. The sun was modeled as a sine function from sunrise to sunset. The model was adjusted to have sunrise at 6:00 am eastern daylight time (EDT) and sunset at 8:30 pm EDT in accordance with the sun's patterns that day, peaking at 12:15 pm EDT. The photolysis rates were provided (Gery et al. 1988). Carter's wall reactions were used to determine the emissions of OH and NO_2 from the interaction of the Teflon walls with the sunlight (Jeffries et al. 1988). The sampling and dilution rates were not provided for the outdoor chamber and therefore were not included in the modeling. Details about the sampling and dilution rates are provided for the rebuilt outdoor smog chamber at UNC, but since this is an updated system it does not represent the dilution rates in 1984, when the data used in this paper was collected.

Sensitivity to Water Vapor

The water vapor profile was unknown for the UNC smog chamber – only the initial and final concentrations were given. Three different water vapor profiles were tested in the model: a constant water vapor concentration at the initial and final concentrations, and a linear variation of water vapor concentration from initial to final, shown in Figure S6 for a linear temperature profile for the toluene case. For most species, the water vapor profile did not make much difference. The biggest difference was for hydrogen peroxide (H_2O_2), but there were not any observational data for this species so the accuracy of the different profiles could not be determined. The linear version was slightly better for ozone prediction and therefore was used in the final profiles shown in Figure S7 and Figure S8.

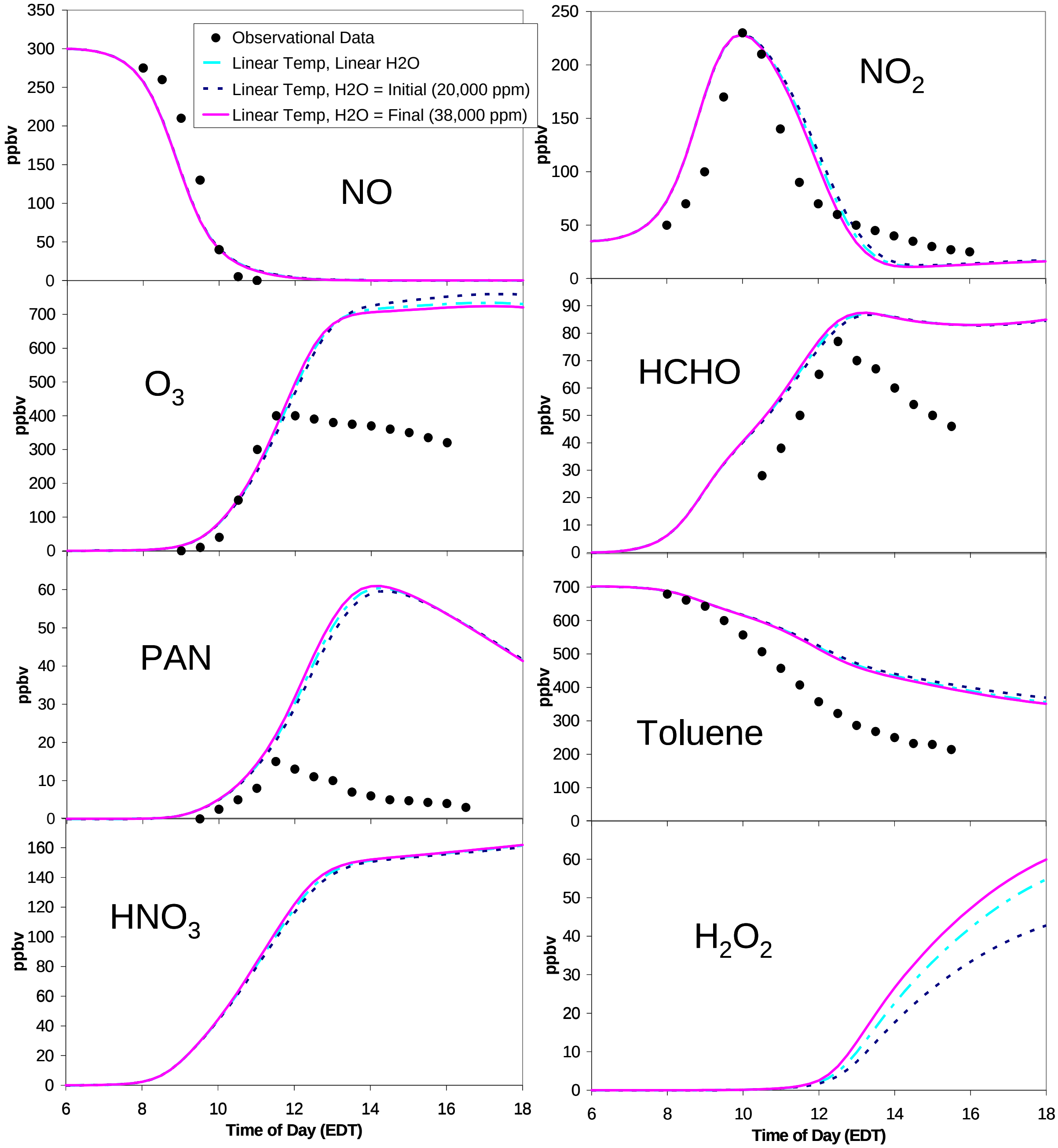

Figure S6: Water Vapor Model Comparisons for Toluene Case using the MCM v. 3.1

Note: Observed Data from Gery et al. (1988)

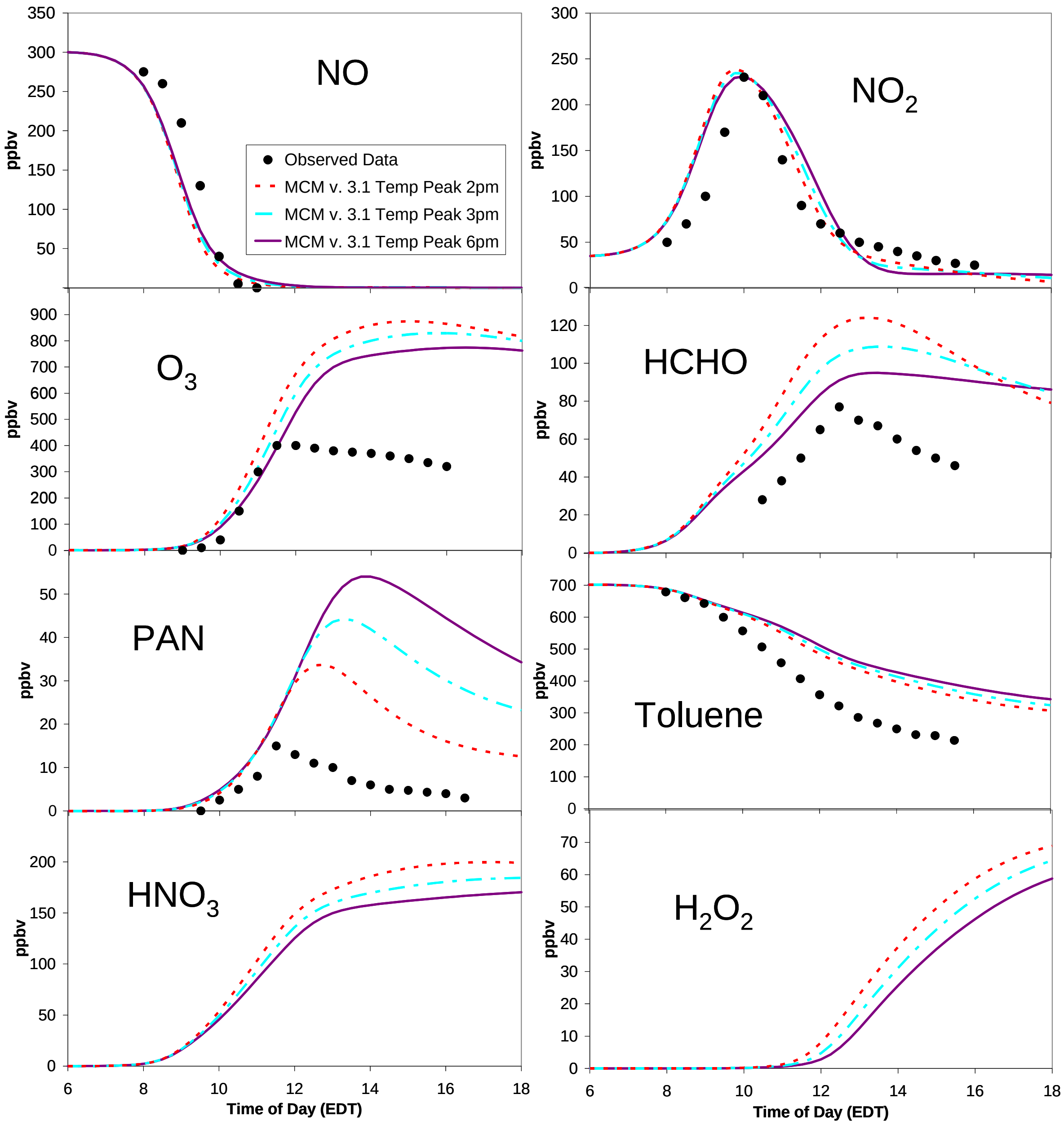

Figure S7: Model Results for MCM v. 3.1 from Three Different Temperature Profiles for Toluene Case

Note: Observed Data from Gery et al. (1988)

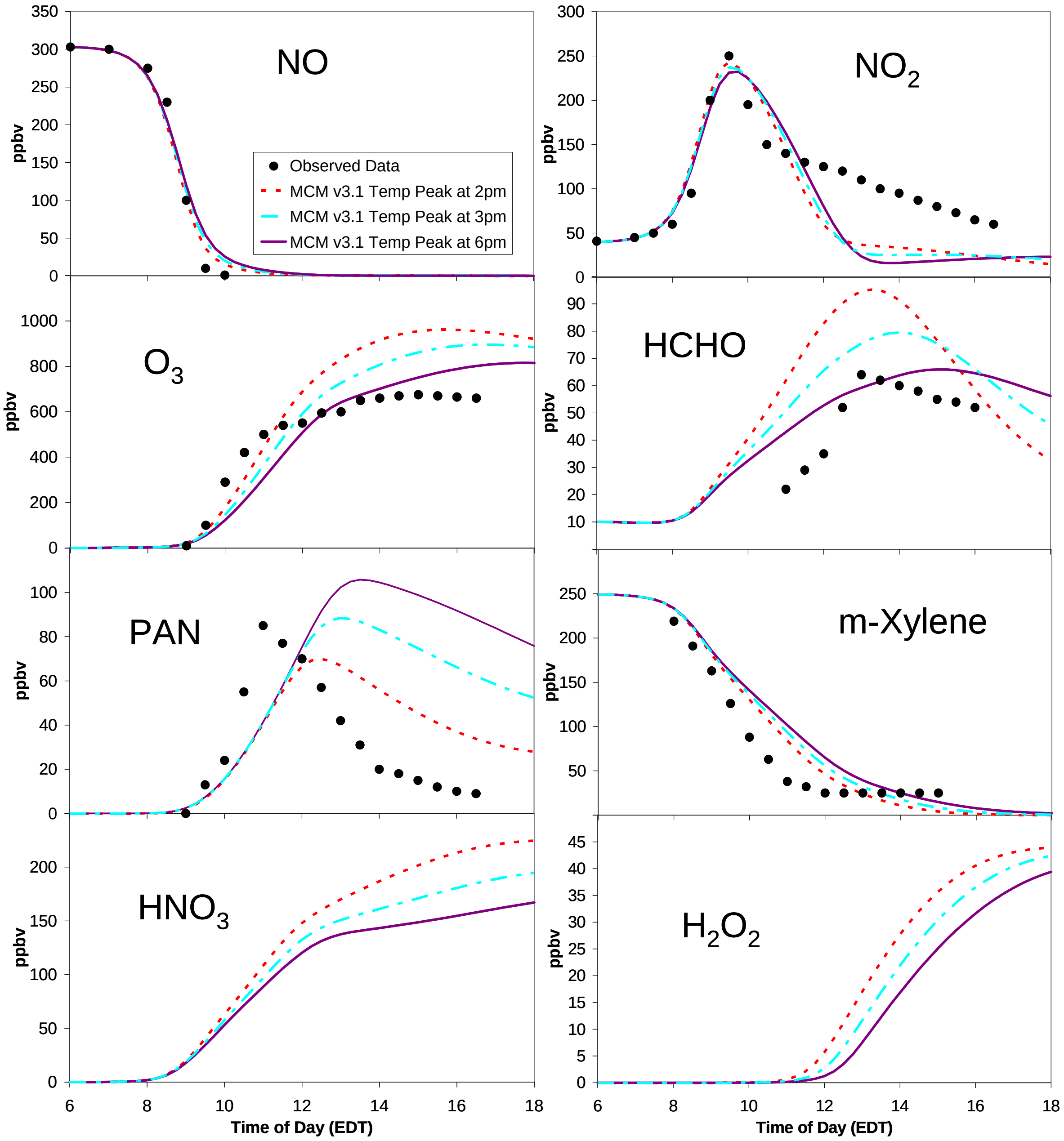

Figure S8: Model Results for MCM v. 3.1 from Three Different Temperature Profiles for m-Xylene Case

Note: Observed Data from Gery et al. (1988)

Sensitivity to Temperature

The model results of some species were sensitive to the temperature in the chamber. The temperature profile was not known for the outdoor chamber. Only the initial and the final temperatures were given, but it is likely that the chamber heated up during the early afternoon and cooled off some in the late afternoon when the final temperature reading was taken. Since the indoor smog chamber model results proved to be very sensitive to the temperature profile, five different temperature profiles were tested for toluene and m-xylene with very different results for some species. Three of the temperature profiles, shown in Figure S9, all have the same initial and final temperatures but have peak temperatures that are different in magnitude and in timing, based on a sine curve. The other two temperature profiles tested and not shown are a linear increase and an average constant temperature. These two scenarios did not match the observed data as well as the sine curve temperature profiles.

The three different temperature profiles based on a sine function were calculated to peak at different times in the afternoon – 2 pm, 3 pm, and 6 pm. The impact these three different temperature profiles had on the model predictions is shown for toluene in Figure S7 and for m-xylene in Figure S8. The impact of temperature on nitric oxide and on organic degradation was minimal. Nitrogen dioxide was only impacted at the low levels after the peak, where the tail trend changed from increasing or flat for the low peak temperature profile to decreasing (more like the observed data) for the higher peak temperature profiles. The predicted trends for other measured species - ozone, formaldehyde, and PAN – were impacted more dramatically, but in different directions. The peak values for ozone and formaldehyde increased when the peak temperature was higher, while the peak value for PAN decreased. The timing of the peaks was also different depending on the timing of the temperature peak. HNO_3 and H_2O_2 were not impacted much in the toluene case but showed more variability with change in temperature in the m-xylene case. The temperature profile is an important parameter when modeling smog chamber data, since it changes the magnitude and timing of predicted peaks for several species.

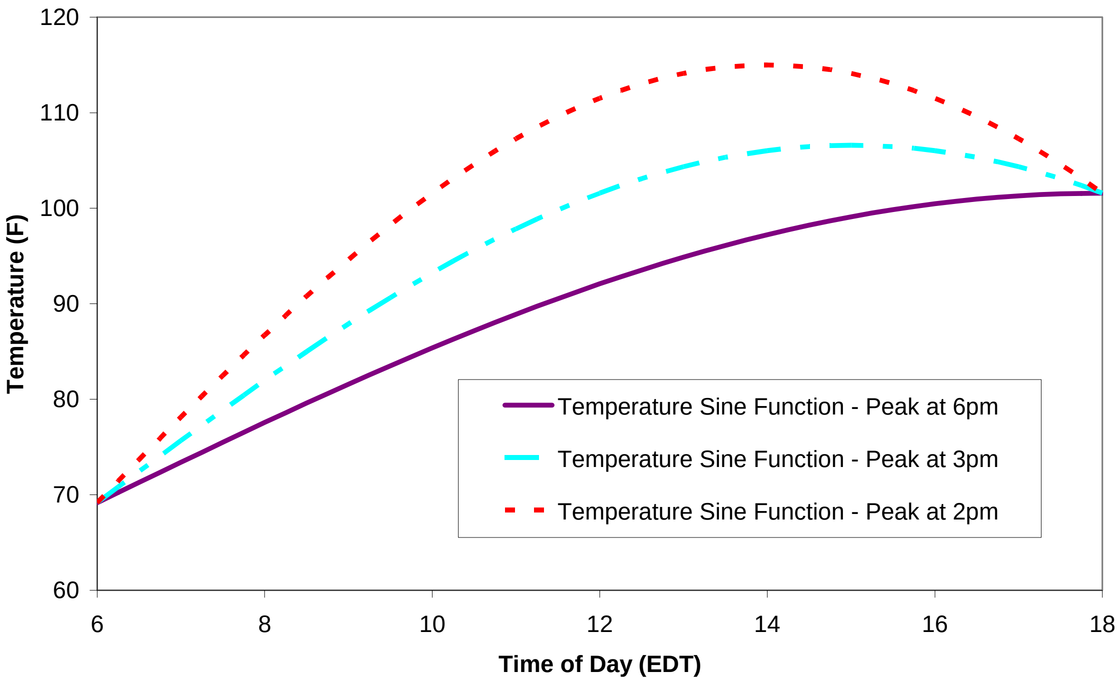

Figure S9: Potential Temperature Profiles for Outdoor Smog Chamber

Toluene Case

As mentioned in the main text, the MCM model predictions for the toluene case overall did not match the observed data so well (Figure S7). The ACBM model was better than the MCM for some species and worse for others (Figure S10). Both models matched the data for NO very well. MCM also matched NO_2 fairly well, but the ACBM model peaked early. The biggest difference between the models was with ozone prediction. The MCM model over-predicted ozone formation by almost double, while the ACBM model under-predicted ozone by 116 ppb. This under-prediction is significant, only capturing 71% of the ozone peak. The timing of the predicted increase in ozone was good for the MCM model while the increase was late for the ACBM model. Both models under-predicted the degradation of toluene. Formaldehyde and PAN were over-predicted in the MCM model by 1.2 to 1.6 times and 2.3 to 3.6 times, respectively, and were very sensitive to changes in the temperature profile. The ACBM model's peak for formaldehyde was early and low, while the PAN trend leveled off at a high value instead of peaking at a lower value like the observed data. HNO_3 and H_2O_2 were only slightly impacted by changes in the temperature profile, but the ACBM model trend for hydrogen peroxide was much lower than in the MCM model. The MCM and ACBM modeled the hydroxyl radical (OH) and hydroperoxy radical (HO_2) similarly for the morning hours while the MCM predicted higher levels in the afternoon than the ACBM.

Differences between data and model results may have been due to sample loss, lighting inconsistencies from the sun, or mechanism inaccuracies. To work on mechanism inaccuracies, the MCM developers at the University of LEEDS are continuing to work on the toluene degradation mechanism because it is known to over-predict ozone formation. In their online training for MCM v. 3.1 (http://mcm.leeds.ac.uk/MCM/tutorial_sec4.htt), they list a tentative alternative mechanism that is under consideration. This modified toluene mechanism was incorporated into the SMVGEAR II model to test the improvements. The results, shown in Figure S10 as MCM v. 3.1 Modified, demonstrate that the mechanism is improving but still needs some work. The ozone, toluene, and formaldehyde predictions improved with the modified toluene mechanism, but the PAN predictions were worse. A recent paper also addresses the toluene mechanism, but it has not been incorporated into the MCM yet (Baltaretu et al. 2009).

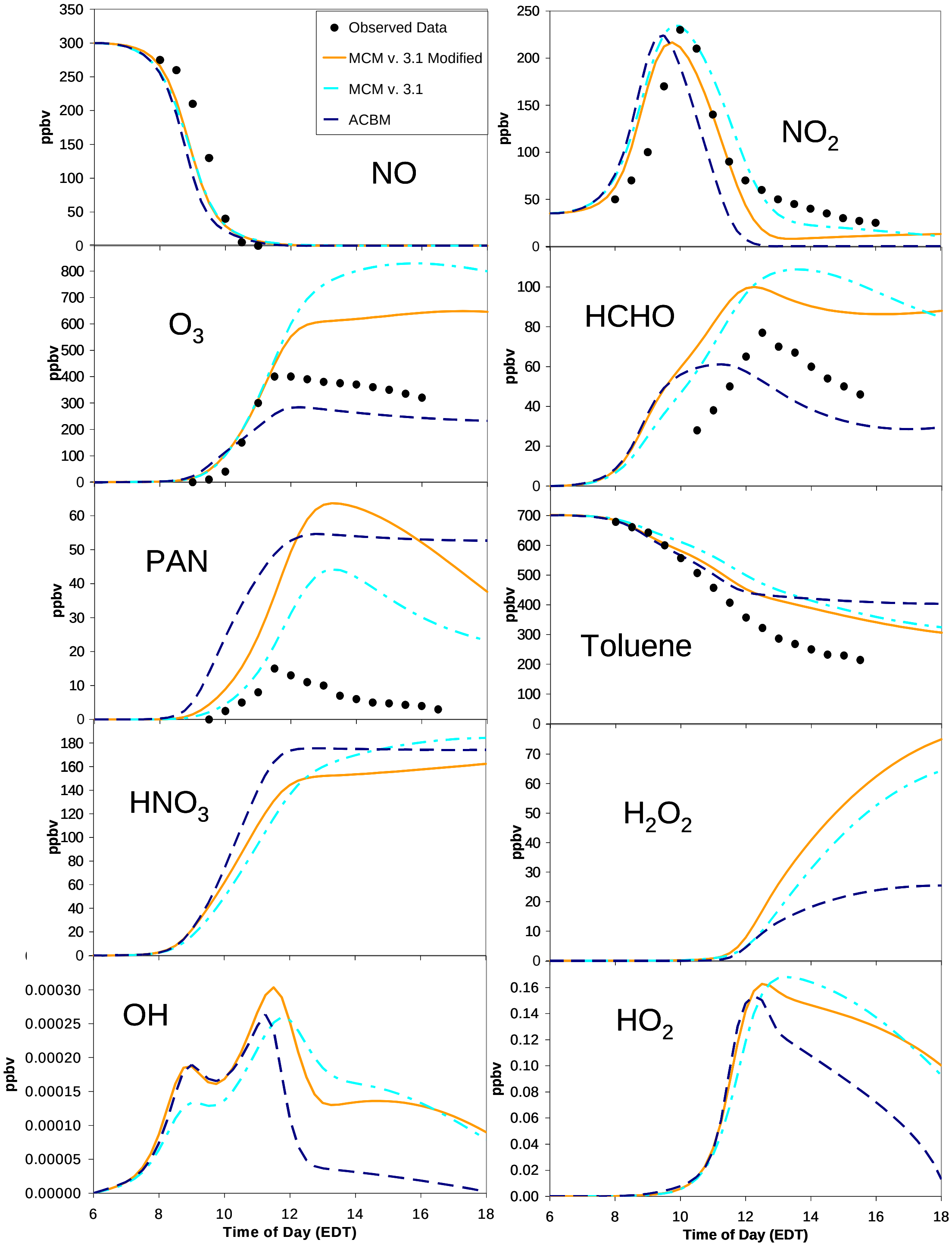

Figure S10: Model Results Comparison for the Toluene Case using MCM v. 3.1, MCM v. 3.1 Modified, and ACBM for the Temperature Profile that Peaks at 3 pm

Note: Observed Data from Gery et al. (1988)

M-Xylene Case

The observed data and the model predictions for the m-xylene case matched fairly well for the MCM, shown in Figure S8. The ACBM treats m-xylene, o-xylene, and p-xylene as one species, XYL (Carter 2008). Since the reaction rates involving the degradation of xylene is an average of these three species in the ACBM instead of explicitly for m-xylene like it is in the MCM, the comparison of the MCM to the ACBM is not discussed. The peak model ozone results using MCM were only 1.3 to 1.5 times the observed peak. The ozone increase was slightly late. The nitrogen oxide curve matched very well. The NO_2 peak was captured by the MCM model but the NO_2 decline after the peak was more gradual than the model results. Similar to the toluene results, the formaldehyde and PAN curves were the correct shape but the peaks were too high and did not align with the measured peak. The predicted degradation of m-xylene was generally in line with the observed data, but the decline was late.

Summary

MCM v. 3.1 was implemented in SMVGEAR II to solve gas-phase atmospheric chemistry. The alkene model results were very good overall, especially for nitric oxide, nitrogen dioxide, and ozone. In most cases, MCM v. 3.1 modeled the data better than did the mixed lumped-explicit ACBM mechanism. The main exception to this was the ozone predictions for the toluene smog chamber scenario when the ACBM performed slightly better than the MCM v. 3.1. SMVGEAR II also sufficiently reduced the computer run times for the MCM to allow it to be modeled in 3-dimensions.

3. Model Setup for E85 Versus Gasoline Comparisons

In this section, the setup of the box model for comparing the effect of E85 versus gasoline and their temperature dependence on gas-phase chemistry is described. Since the emissions data were based on data from Jacobson's study (2007a; 2007b), summarized in Table S4, the first step was to determine the emissions for gasoline and for E85 with more explicit treatment than was used for the ACBM. To do this, we used data from Black (1995-1997), which gives the speciated exhaust emissions for reformulated gasoline (RFG) in a Ford Taurus and for ethanol (E85) in a Ford Lumina Flex Fuel Vehicle (FFV) during the first 124 seconds of cold start. The data are summarized in Table S5.

We assumed that the speciation during a cold start is similar to that during the whole vehicle cycle, but the emission amounts differ because larger amounts of unburned emissions occur during cold start than during the whole driving cycle. The actual emissions are based on emissions data for current gasoline vehicles for the South Coast Air Basin (SCAB), moved forward to the year 2020, shown in Table S4. We assume that all of the vehicles change from gasoline to E85. The results can then be applied to any situation where a change is being made from gasoline to E85.

To start separating the emissions data from Table S4 into more explicit species, we first used the Black emissions data for RFG and E85 to determine the % of total organic gases (TOG) for each emitted species in the Black data, shown in Table S5. Unfortunately, there were many species measured whose chemical nature was not discernable. These species were lumped together and assumed to be unreactive. There were also some species in the Black data not included in the MCM, but this was a small fraction of the total amount of species in the emissions. Even though the MCM is a near-explicit chemical mechanism, it does not describe the degradation of all organic species (that would be impractical) – it concentrates on commonly-emitted species. For the ethanol (E85) emissions, the known species from Black's data that also existed in the MCM made up a large portion (over 95%) of the TOG measured. For RFG, the known species from the data that were in the MCM made up about 75% of the TOG measured.

To include more of the known species in the MCM model, information about the reactivity of species from Carter's carbon bond mechanism was used (Carter 2008).

		Emissions Data (tonnes/yr)		
Species	**In Model**	**Gasoline**	**% Change**	**E-85 Replacing All Gasoline**
CO	CO	782,000	5%	821,100
NOx		68,900	-30%	48,230
NO2	NO2	62,010		43,407
NO	NO	6,201		4,341
Methane	CH4	8,530	43%	12,198
Ethane	C2H6	1,220	0%	1,220
Propane	C3H8	465	-65%	163
Paraffin bond group	PAR	44,720	-80%	8,944
Ethene	C2H4	3,570	-17%	2,963
Propene	C3H6	988	-65%	346
1,3 Butadiene	C4H6	1,390	-10%	1,251
Olefin bond group	OLE	949	-17%	788
Methanol	CH3OH	-	0%	-
Ethanol	C2H5OH	-	0%	69,800
Formaldehyde	HCHO	650	60%	1,040
Acetaldehyde		232	2000%	4,872
Higher Aldehydes		3,460	-60%	1,384
Acetaldehyde plus higher	CH3CHO	3,692	1940%	6,256
Formic Acid		-	0%	-
Acetic acid		-	0%	-
Acetone		-	0%	-
Benzene	C6H6	1,270	-79%	267
Toluene bond group	TOL	6,260	-80%	1,252
Xylene bond group	XYL	11,600	-80%	2,320
Isoprene bond group	ISOP	65	-80%	13
Unreactive		4,540	-80%	908
Total organic gas		89,909		109,728

Table S4: Emissions Data for Gasoline and E85 (Jacobson 2007a)

Note: The gasoline emissions data was brought forward to the year 2020 by calculating it as 40% of the 2002 emissions for the South Coast Air Basin, (EPA 2006; Jacobson 2007a). The percent change between gasoline and E85 (where a positive change means an increase in emissions for E85) are compiled results of 12 different studies on emissions from E85 (Jacobson 2007a).

Compound	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)	Taurus RFG (% of total NMOG)	Lumina FFV E85 (% of total NMOG)	**Taurus RFG (% of TOG)**	**Lumina FFV E85 (% of TOG)**	MCM species name
NMOG							
Alkanes	33.446	13.222	37%	10%	**35%**	**9%**	
Alkenes	17.281	15.07	19%	12%	**18%**	**11%**	
Aromatics	29.666	7.929	33%	6%	**31%**	**6%**	
Alkynes	3.588	2.142	4%	2%	**4%**	**1%**	
Unknowns	0.338	0.077	0%	0%	**0%**	**0%**	
Alcohols/Ethers	3.627	74.956	4%	59%	**4%**	**52%**	
Aldehydes/Ketones	2.683	14.414	3%	11%	**3%**	**10%**	
Total NMOG	**90.628**	**127.81**	100%	100%	**95%**	**89%**	
Methane	**5.025**	**15.708**			**5%**	**11%**	
CO	**393.7**	**510.117**					
TOG	**95.653**	**143.518**			**100%**	**100%**	
TOG in MCM	71.816	136.447			**75.08%**	**95.07%**	
TOG not in MCM	23.837	7.071					
Methane	5.025	15.708			**5.25%**	**10.94%**	**CH4**
Ethylene (ethene)	4.991	10.799	5.51%	8.45%	**5.22%**	**7.52%**	**C2H4**
Ethane	1.26	2.255	1.39%	1.76%	**1.32%**	**1.57%**	**C2H6**
Acetylene	3.103	1.936	3.42%	1.51%	**3.24%**	**1.35%**	**C2H2**
Propylene	3.284	1.046	3.62%	0.82%	**3.43%**	**0.73%**	**C3H6**
Iso-butane	0.022	0.02	0.02%	0.02%	**0.02%**	**0.01%**	**IC4H10**
1-Butene	0	0.294	0.00%	0.23%	**0.00%**	**0.20%**	**BUT1ENE**
Iso-Butylene	4.313	0.548	4.76%	0.43%	**4.51%**	**0.38%**	**MEPROPENE**
1,3 Butadiene	0.507	0.067	0.56%	0.05%	**0.53%**	**0.05%**	**C4H6**
N-Butane	0.338	0.969	0.37%	0.76%	**0.35%**	**0.68%**	**NC4H10**
Trans-2-Butene	0.335	0.156	0.37%	0.12%	**0.35%**	**0.11%**	**TBUT2ENE**
Cis-2-Butene	0.246	0.681	0.27%	0.53%	**0.26%**	**0.47%**	**CBUT2ENE**
3-Methyl-1-Butene	0.114	0.03	0.13%	0.02%	**0.12%**	**0.02%**	**ME3BUT1ENE**
Iso-Pentane	4.658	1.434	5.14%	1.12%	**4.87%**	**1.00%**	**IC5H12**
1-Pentene	0.135	0.044	0.15%	0.03%	**0.14%**	**0.03%**	**PENT1ENE**
2-Methyl-1-butene	0.203	0.067	0.22%	0.05%	**0.21%**	**0.05%**	**ME2BUT1ENE**
N-pentane	0.817	0.639	0.90%	0.50%	**0.85%**	**0.45%**	**NC5H12**
C5H8 TOTAL	0.147	0.044	0.16%	0.03%	**0.15%**	**0.05%**	**C5H8**
isoprene	0.122	0.022	0.13%	0.02%	0.13%	0.03%	
C5H8	0.01	0.006	0.01%	0.00%	0.01%	0.00%	
c5h8	0.015	0.016	0.02%	0.01%	0.02%	0.01%	
trans-2-pentene	0.235	0.064	0.26%	0.05%	**0.25%**	**0.04%**	**TPENT2ENE**
cis-2-pentene	0.123	0.037	0.14%	0.03%	**0.13%**	**0.03%**	**CPENT2ENE**
2-methyl-2-butene	0.103	0.063	0.11%	0.05%	**0.11%**	**0.04%**	**ME2BUT2ENE**
2,2-dimethylbutane	0.307	0.111	0.34%	0.09%	**0.32%**	**0.08%**	**M22C4**
2,3-dimethylbutane	0.882	0.28	0.97%	0.22%	**0.92%**	**0.20%**	**M23C4**
2-methylpentane	2.179	0.766	2.40%	0.60%	**2.28%**	**0.53%**	**M2PE**
3-methylpentane	1.252	0.353	1.38%	0.28%	**1.31%**	**0.25%**	**M3PE**
1-Hexene	0.081	0.036	0.09%	0.03%	**0.08%**	**0.03%**	**HEX1ENE**
N-Hexane	0.64	0.386	0.71%	0.30%	**0.67%**	**0.27%**	**NC6H14**
trans-2-hexene	0.104	0.039	0.11%	0.03%	**0.11%**	**0.03%**	**THEX2ENE**
cis-2-hexene	0.049	0.019	0.05%	0.01%	**0.05%**	**0.01%**	**CHEX2ENE**
2,3-dimethyl-2-butene	0.028	0.009	0.03%	0.01%	**0.03%**	**0.01%**	**DM23BU2ENE**
benzene	3.229	1.071	3.56%	0.84%	**3.38%**	**0.75%**	**BENZENE**
cyclohexane	0	0.023	0.00%	0.02%	**0.00%**	**0.02%**	**CHEX**
2-methylhexane	1.065	0.233	1.18%	0.18%	**1.11%**	**0.16%**	**M2HEX**
3-methylhexane	1.146	0.251	1.26%	0.20%	**1.20%**	**0.17%**	**M3HEX**
n-heptane	0.668	0.165	0.74%	0.13%	**0.70%**	**0.11%**	**NC7H16**
toluene	7.688	2.273	8.48%	1.78%	**8.04%**	**1.58%**	**TOLUENE**
n-octane	0.276	0.091	0.30%	0.07%	**0.29%**	**0.06%**	**NC8H18**
ethylbenzene	2.412	0.731	2.66%	0.57%	**2.52%**	**0.51%**	**EBENZ**
M&P-Xylene	5.868	1.621	6.47%	1.27%	**6.13%**	**1.13%**	**MXYL, PXYL**
styrene	0.455	0.079	0.50%	0.06%	**0.48%**	**0.06%**	**STYRENE**
o-xylene	2.15	0.518	2.37%	0.41%	**2.25%**	**0.36%**	**OXYL**
n-nonane	0.105	0.023	0.12%	0.02%	**0.11%**	**0.02%**	**NC9H20**
isopropylbenzene	0.108	0.031	0.12%	0.02%	**0.11%**	**0.02%**	**IPBENZ**
n-propylbenzene	0.386	0.066	0.43%	0.05%	**0.40%**	**0.05%**	**PBENZ**
1-methyl-3-ethylbenzene	1.474	0.298	1.63%	0.23%	**1.54%**	**0.21%**	**METHTOL**
1-methyl-4-ethylbenzene	0.661	0.131	0.73%	0.10%	**0.69%**	**0.09%**	**PETHTOL**
1,3,5-trimethylbenzene	0.739	0.193	0.82%	0.15%	**0.77%**	**0.13%**	**TM135B**
1-methyl-2-ethylbenzene	0.476	0.094	0.53%	0.07%	**0.50%**	**0.07%**	**OETHTOL**
1,2,4-trimethylbenzene	1.658	0.337	1.83%	0.26%	**1.73%**	**0.23%**	**TM124B**
n-decane	0.037	0.007	0.04%	0.01%	**0.04%**	**0.00%**	**NC10H22**
1,2,3-trimethylbenzene	0.008	0.063	0.01%	0.05%	**0.01%**	**0.04%**	**TM123B**
1,3-dimethyl-5-ethylbenzene	0.056	0.002	0.06%	0.00%	**0.06%**	**0.00%**	**DIME35EB**
n-undecane	0.012	0.004	0.01%	0.00%	**0.01%**	**0.00%**	**NC11H24**
n-dodecane	0.007	0.001	0.01%	0.00%	**0.01%**	**0.00%**	**NC12H26**
mtbe	3.06	0.922	3.38%	0.72%	**3.20%**	**0.64%**	**MTBE**

Compound (continued)	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)	Taurus RFG (% of total NMOG)	Lumina FFV E85 (% of total NMOG)	**Taurus RFG (% of TOG)**	**Lumina FFV E85 (% of TOG)**	MCM species name
methanol	0.229	6.684	0.25%	5.23%	**0.24%**	**4.66%**	**CH3OH**
ethanol	0.026	67.309	0.03%	52.66%	**0.03%**	**46.90%**	**C2H5OH**
2-propanol	0.312	0.04	0.34%	0.03%	**0.33%**	**0.03%**	**IPROPOL**
formaldehyde	0.605	1.528	0.67%	1.20%	**0.63%**	**1.06%**	**HCHO**
acetaldehyde	0.389	12.447	0.43%	9.74%	**0.41%**	**8.67%**	**CH3CHO**
acetone	0.461	0.121	0.51%	0.09%	**0.48%**	**0.08%**	**CH3COCH3**
propionaldehyde	0.095	0.064	0.10%	0.05%	**0.10%**	**0.04%**	**C2H5CHO**
butyraldehyde	0.063	0	0.07%	0.00%	**0.07%**	**0.00%**	**C3H7CHO**
benzaldehyde	0.255	0.088	0.28%	0.07%	**0.27%**	**0.06%**	**BENZAL**
x-butyraldehyde	0.044	0	0.05%	0.00%	**0.05%**	**0.00%**	**IPRCHO**
x-valeraldehyde	0.047	0.007	0.05%	0.01%	**0.05%**	**0.00%**	**C4H9CHO**
2-butanone	0.065	0.031	0.07%	0.02%	**0.07%**	**0.02%**	**MEK**
2,4-dimethylpentane	1.374	0.416	1.52%	0.33%	**1.44%**	**0.29%**	
2,3-dimethylpentane	2.844	0.74	3.14%	0.58%	**2.97%**	**0.52%**	
iso-octane	5.026	1.561	5.55%	1.22%	**5.25%**	**1.09%**	
methylcyclopentane	0.54	0.193	0.60%	0.15%	**0.56%**	**0.13%**	
2,3,4-trimethylpentane	1.459	0.4	1.61%	0.31%	**1.53%**	**0.28%**	
Propadiene	0.055	0.019	0.06%	0.01%	**0.06%**	**0.01%**	
Methylacetylene	0.29	0.038	0.32%	0.03%	**0.30%**	**0.03%**	
1-Buten-3-yne	0.126	0	0.14%	0.00%	**0.13%**	**0.00%**	
1-Butyne	0.021	0.105	0.02%	0.08%	**0.02%**	**0.07%**	
1,3-Butadiyne	0.028	0.003	0.03%	0.00%	**0.03%**	**0.00%**	
1,2-Butadiene	0.024	0.002	0.03%	0.00%	**0.03%**	**0.00%**	
1,4-Pentadiene	0.006	0.118	0.01%	0.09%	**0.01%**	**0.08%**	
2-Butyne	0.013	0.057	0.01%	0.04%	**0.01%**	**0.04%**	
2-Methyl-1-buten-3-yne	0.008	0.003	0.01%	0.00%	**0.01%**	**0.00%**	
3,3-dimethyl-1-butene	0.015	0.009	0.02%	0.01%	**0.02%**	**0.01%**	
trans-1,3-pentadiene	0.034	0.008	0.04%	0.01%	**0.04%**	**0.01%**	
cyclopentadiene	0.003	0.005	0.00%	0.00%	**0.00%**	**0.00%**	
cis-1,3-pentadiene	0.002	0.018	0.00%	0.01%	**0.00%**	**0.01%**	
cyclopentene	0.048	0.035	0.05%	0.03%	**0.05%**	**0.02%**	
3-methyl-1-pentene	0.167	0.065	0.18%	0.05%	**0.17%**	**0.05%**	
cyclopentane	0.072	0.043	0.08%	0.03%	**0.08%**	**0.03%**	
4-methyl-cis-2-pentene	0	0.007	0.00%	0.01%	**0.00%**	**0.00%**	
4-methyl-trans-2-pentene	0.104	0.043	0.11%	0.03%	**0.11%**	**0.03%**	
2-methyl-1-pentene	0.05	0.022	0.06%	0.02%	**0.05%**	**0.02%**	
2-Ethyl-1-Butene	0.002	0.001	0.00%	0.00%	**0.00%**	**0.00%**	
Cis-3-hexene	0.05	0.018	0.06%	0.01%	**0.05%**	**0.01%**	
trans-3-hexene	0.013	0.004	0.01%	0.00%	**0.01%**	**0.00%**	
2-methyl-2-pentene	0.056	0.034	0.06%	0.03%	**0.06%**	**0.02%**	
3-methylcyclopentene	0.034	0.014	0.04%	0.01%	**0.04%**	**0.01%**	
cis-3-methyl-2-pentene	0.035	0.021	0.04%	0.02%	**0.04%**	**0.01%**	
4-methylcyclopentene	0.018	0.009	0.02%	0.01%	**0.02%**	**0.01%**	
trans-3-methyl-2-pentene	0.053	0.031	0.06%	0.02%	**0.06%**	**0.02%**	
2,2-dimethylpentane	0.087	0.021	0.10%	0.02%	**0.09%**	**0.01%**	
2,2,3-trimethylbutane	0.041	0.023	0.05%	0.02%	**0.04%**	**0.02%**	
2,4-dimethyl-1-pentene	0.034	0.01	0.04%	0.01%	**0.04%**	**0.01%**	
1-methylcyclopentene	0.037	0.029	0.04%	0.02%	**0.04%**	**0.02%**	
4,4-dimethyl-2-pentene	0.056	0.018	0.06%	0.01%	**0.06%**	**0.01%**	
3,3-dimethylpentane	0.092	0.02	0.10%	0.02%	**0.10%**	**0.01%**	
trans-2-methyl-3-hexene	0.029	0.005	0.03%	0.00%	**0.03%**	**0.00%**	
4-methyl-1-hexene	0.019	0.006	0.02%	0.00%	**0.02%**	**0.00%**	
1,1-dimethylcyclopentane	0.039	0.024	0.04%	0.02%	**0.04%**	**0.02%**	
trans-5-methyl-2-hexene	0.024	0.008	0.03%	0.01%	**0.03%**	**0.01%**	
cis-1,3-dimethylcyclopentane	0.167	0.041	0.18%	0.03%	**0.17%**	**0.03%**	
trans-1,3-dimethylcyclopentane	0.282	0.067	0.31%	0.05%	**0.29%**	**0.05%**	
3-methyl-trans-3-hexene	0.013	0.006	0.01%	0.00%	**0.01%**	**0.00%**	
trans-3-heptene	0.042	0.014	0.05%	0.01%	**0.04%**	**0.01%**	
cis-3-methyl-3-hexene	0.097	0.037	0.11%	0.03%	**0.10%**	**0.03%**	
trans-2-heptene	0.042	0.014	0.05%	0.01%	**0.04%**	**0.01%**	
3-ethyl-2-pentene	0.041	0.007	0.05%	0.01%	**0.04%**	**0.00%**	
2-methyl-2-hexene	0.034	0.029	0.04%	0.02%	**0.04%**	**0.02%**	
1,5-dimethylcycleopentene	0.049	0.021	0.05%	0.02%	**0.05%**	**0.01%**	
2,3-dimethyl-2-pentene	0.014	0.001	0.02%	0.00%	**0.01%**	**0.00%**	
3-ethyl cyclopentene	0.006	0.003	0.01%	0.00%	**0.01%**	**0.00%**	
4-ethyl cyclopentene	0.01	0.004	0.01%	0.00%	**0.01%**	**0.00%**	
1-cis-2-dimethylcyclopentane	0.104	0.033	0.11%	0.03%	**0.11%**	**0.02%**	
methylcyclohexane	0.217	0.068	0.24%	0.05%	**0.23%**	**0.05%**	
1,1,3-trimethylcyclopentane	0.02	0.011	0.02%	0.01%	**0.02%**	**0.01%**	
2,5-dimethylhexane	0.4	0.124	0.44%	0.10%	**0.42%**	**0.09%**	
2,4-dimethylhexane	0.757	0.196	0.84%	0.15%	**0.79%**	**0.14%**	c8h18
2,2,3-trimethylpentane	0.008	0.036	0.01%	0.03%	**0.01%**	**0.03%**	
3-methylcyclohexene	0.015	0.007	0.02%	0.01%	**0.02%**	**0.00%**	
4-methylcyclohexene	0.005	0.003	0.01%	0.00%	**0.01%**	**0.00%**	
1,2,4-trimethylcyclopentane	0.073	0.027	0.08%	0.02%	**0.08%**	**0.02%**	
c,t,c-1,2,3-trimethylcyclopentane	0.025	0.01	0.03%	0.01%	**0.03%**	**0.01%**	
1-ethylcyclopentene	0	0.008	0.00%	0.01%	**0.00%**	**0.01%**	

Compound (continued)	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)	Taurus RFG (% of total NMOG)	Lumina FFV E85 (% of total NMOG)	**Taurus RFG (% of TOG)**	**Lumina FFV E85 (% of TOG)**	MCM species name
2,3-dimethylhexane	0.502	0.149	0.55%	0.12%	**0.52%**	**0.10%**	c8h18
2-methylheptane	0.339	0.111	0.37%	0.09%	**0.35%**	**0.08%**	
4-methylheptane	0.158	0.055	0.17%	0.04%	**0.17%**	**0.04%**	
3,4-dimethylhexane	0.129	0.046	0.14%	0.04%	**0.13%**	**0.03%**	
3-methylheptane	0.383	0.127	0.42%	0.10%	**0.40%**	**0.09%**	
3-ethylhexane	0.074	0.027	0.08%	0.02%	**0.08%**	**0.02%**	
1,2,4-trimethylcyclopentane	0.031	0.01	0.03%	0.01%	**0.03%**	**0.01%**	
trans-1,4-dimethylcyclohexane	0.089	0.022	0.10%	0.02%	**0.09%**	**0.02%**	
2,2,5-trimethylhexane	0.551	0.205	0.61%	0.16%	**0.58%**	**0.14%**	C9H20
1-octene	0.022	0.01	0.02%	0.01%	**0.02%**	**0.01%**	
trans-1-ethyl-3-methylcyclopentane	0.009	0.002	0.01%	0.00%	**0.01%**	**0.00%**	
cis-1-ethyl-3-methylcyclopentane	0.056	0.016	0.06%	0.01%	**0.06%**	**0.01%**	
1,1,2-trimethylcyclopentane	0.021	0.007	0.02%	0.01%	**0.02%**	**0.00%**	
1,2,3-trimethylcyclopentane	0.017	0.006	0.02%	0.00%	**0.02%**	**0.00%**	
2-octene	0	0.003	0.00%	0.00%	**0.00%**	**0.00%**	
isopropylcyclopentane	0.091	0.011	0.10%	0.01%	**0.10%**	**0.01%**	
2,3,5-trimethylhexane	0.107	0.04	0.12%	0.03%	**0.11%**	**0.03%**	
2,4-dimethylheptane	0.063	0.018	0.07%	0.01%	**0.07%**	**0.01%**	
2,6-dimethylheptane	0.067	0.019	0.07%	0.01%	**0.07%**	**0.01%**	
2,5-dimethylheptane	0.14	0.04	0.15%	0.03%	**0.15%**	**0.03%**	
3,5-dimethylheptane	0.064	0.021	0.07%	0.02%	**0.07%**	**0.01%**	
1,1,4-trimethylcyclohexane	0.009	0	0.01%	0.00%	**0.01%**	**0.00%**	
3,4-dimethylheptane	0.069	0.017	0.08%	0.01%	**0.07%**	**0.01%**	
3-methyloctane	0.179	0.045	0.20%	0.04%	**0.19%**	**0.03%**	
1-nonene	0	0.007	0.00%	0.01%	**0.00%**	**0.00%**	
n-butylcyclopentane	0	0.001	0.00%	0.00%	**0.00%**	**0.00%**	
o-methylstyrene	0.172	0.021	0.19%	0.02%	**0.18%**	**0.01%**	
2-methylpropylbenzene	0.034	0.008	0.04%	0.01%	**0.04%**	**0.01%**	
1-methylprobylbenzene	0.023	0.007	0.03%	0.01%	**0.02%**	**0.00%**	
1-methyl-3-isopropylbenzene	0.038	0.009	0.04%	0.01%	**0.04%**	**0.01%**	
p-methylstyrene	0.223	0	0.25%	0.00%	**0.23%**	**0.00%**	
2,3-dihydroindene(indan)	0.081	0.043	0.09%	0.03%	**0.08%**	**0.03%**	
1,3-diethylbenzene	0.15	0.04	0.17%	0.03%	**0.16%**	**0.03%**	
1-methyl-3-n-propylbenzene	0.33	0.034	0.36%	0.03%	**0.34%**	**0.02%**	
1,2-diethylbenzene	0.055	0.069	0.06%	0.05%	**0.06%**	**0.05%**	
1-methyl-2-n-propylbenzene	0.006	0.011	0.01%	0.01%	**0.01%**	**0.01%**	
1,4-dimethyl-2-ethylbenzene	0.059	0	0.07%	0.00%	**0.06%**	**0.00%**	
1,3-dimethyl-4-ethylbenzene	0.09	0.02	0.10%	0.02%	**0.09%**	**0.01%**	
1,2-dimethyl-4-ethylbenzene	0.116	0.02	0.13%	0.02%	**0.12%**	**0.01%**	
o-ethylstyrene	0.065	0.001	0.07%	0.00%	**0.07%**	**0.00%**	
1,3-dimethyl-2-ethylbenzene	0.051	0.035	0.06%	0.03%	**0.05%**	**0.02%**	
m-ethylstyrene	0.073	0	0.08%	0.00%	**0.08%**	**0.00%**	
1,2-dimethyl-3-ethylbenzene	0.005	0.006	0.01%	0.00%	**0.01%**	**0.00%**	
1,2,4,5-tetramethylbenzene	0.095	0.011	0.10%	0.01%	**0.10%**	**0.01%**	
1,2,3,5-tetramethylbenzene	0.025	0.016	0.03%	0.01%	**0.03%**	**0.01%**	
1-methyl-1h-idene	0.039	0	0.04%	0.00%	**0.04%**	**0.00%**	
naphthalene	0.135	0.021	0.15%	0.02%	**0.14%**	**0.01%**	
acrolein	0.04	0.013	0.04%	0.01%	**0.04%**	**0.01%**	
crotonaldehyde	0.022	0	0.02%	0.00%	**0.02%**	**0.00%**	
o-tolualdehyde	0.076	0	0.08%	0.00%	**0.08%**	**0.00%**	
m-tolualdehyde	0.173	0.029	0.19%	0.02%	**0.18%**	**0.02%**	
p-tolualdehyde	0.093	0	0.10%	0.00%	**0.10%**	**0.00%**	
2,5-dmbenzaldehyde	0.01	0	0.01%	0.00%	**0.01%**	**0.00%**	
x-dmbenzaldehyde	0.038	0	0.04%	0.00%	**0.04%**	**0.00%**	
x-acrolein	0.091	0.057	0.10%	0.04%	**0.10%**	**0.04%**	
methacrolein	0.118	0.031	0.13%	0.02%	**0.12%**	**0.02%**	
c6h10	0.01	0.005	0.01%	0.00%	**0.01%**	**0.00%**	
c6h8	0.004	0.002	0.00%	0.00%	**0.00%**	**0.00%**	
C7H12 TOTAL	0.035	0.008	0.04%	0.01%	**0.04%**	**0.01%**	
c7h12	0.014	0.005	0.02%	0.00%	**0.01%**	**0.00%**	
c7h12	0.021	0.003	0.02%	0.00%	**0.02%**	**0.00%**	
c7h14	0.105	0.066	0.12%	0.05%	**0.11%**	**0.05%**	
C8H14 TOTAL	0.108	0.041	0.12%	0.03%	**0.11%**	**0.03%**	
c8h14	0.018	0.01	0.02%	0.01%	**0.02%**	**0.01%**	
c8h14	0.046	0.018	0.05%	0.01%	**0.05%**	**0.01%**	
c8h14	0.012	0.004	0.01%	0.00%	**0.01%**	**0.00%**	
c8h14	0.032	0.009	0.04%	0.01%	**0.03%**	**0.01%**	
C8H16 TOTAL	0.254	0.07	0.28%	0.05%	**0.27%**	**0.05%**	
c8h16	0.013	0.004	0.01%	0.00%	**0.01%**	**0.00%**	
c8h16	0.072	0.018	0.08%	0.01%	**0.08%**	**0.01%**	
c8h16	0.067	0.02	0.07%	0.02%	**0.07%**	**0.01%**	
c8h16	0.021	0.006	0.02%	0.00%	**0.02%**	**0.00%**	
c8h16	0.081	0.022	0.09%	0.02%	**0.08%**	**0.02%**	

Compound (continued)	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)	Taurus RFG (% of total NMOG)	Lumina FFV E85 (% of total NMOG)	**Taurus RFG (% of TOG)**	**Lumina FFV E85 (% of TOG)**	MCM species name
C9H18 TOTAL	0.454	0.115	0.50%	0.09%	**0.47%**	**0.08%**	
c9h18	0.021	0.006	0.02%	0.00%	**0.02%**	**0.00%**	
c9h18	0.041	0.01	0.05%	0.01%	**0.04%**	**0.01%**	
c9h18	0.018	0.003	0.02%	0.00%	**0.02%**	**0.00%**	
c9h18	0.047	0.013	0.05%	0.01%	**0.05%**	**0.01%**	
c9h18	0.004	0	0.00%	0.00%	**0.00%**	**0.00%**	
c9h18	0.105	0.037	0.12%	0.03%	**0.11%**	**0.03%**	
c9h18	0.019	0.001	0.02%	0.00%	**0.02%**	**0.00%**	
c9h18	0.014	0.002	0.02%	0.00%	**0.01%**	**0.00%**	
c9h18	0.057	0.012	0.06%	0.01%	**0.06%**	**0.01%**	
c9h18	0.061	0.02	0.07%	0.02%	**0.06%**	**0.01%**	
c9h18	0.037	0.007	0.04%	0.01%	**0.04%**	**0.00%**	
c9h18	0.03	0.004	0.03%	0.00%	**0.03%**	**0.00%**	
c9h16	0.033	0.008	0.04%	0.01%	**0.03%**	**0.01%**	
C10H22 TOTAL	0.37	0.084	0.41%	0.07%	**0.39%**	**0.06%**	
c10h22	0.102	0.034	0.11%	0.03%	**0.11%**	**0.02%**	
c10h22 ?	0.03	0.006	0.03%	0.00%	**0.03%**	**0.00%**	
c10h22 ?	0.038	0.005	0.04%	0.00%	**0.04%**	**0.00%**	
c10h22 ?	0.015	0.003	0.02%	0.00%	**0.02%**	**0.00%**	
c10h22 ?	0.05	0.014	0.06%	0.01%	**0.05%**	**0.01%**	
c10h22 ?	0.026	0.005	0.03%	0.00%	**0.03%**	**0.00%**	
c10h22	0.045	0.007	0.05%	0.01%	**0.05%**	**0.00%**	
c10h22	0.064	0.01	0.07%	0.01%	**0.07%**	**0.01%**	
C10H20 TOTAL	0.186	0.055	0.21%	0.04%	**0.19%**	**0.04%**	
c10h20	0.013	0.001	0.01%	0.00%	**0.01%**	**0.00%**	
c10h20	0.025	0.012	0.03%	0.01%	**0.03%**	**0.01%**	
c10h20	0.01	0.021	0.01%	0.02%	**0.01%**	**0.01%**	
c10h20	0.008	0.005	0.01%	0.00%	**0.01%**	**0.00%**	
c10h20	0.015	0.004	0.02%	0.00%	**0.02%**	**0.00%**	
c10h20	0.024	0.01	0.03%	0.01%	**0.03%**	**0.01%**	
c10h20	0.016	0.002	0.02%	0.00%	**0.02%**	**0.00%**	
c10h20	0.075	0	0.08%	0.00%	**0.08%**	**0.00%**	
C11H24 TOTAL	0.316	0.014	0.35%	0.01%	**0.33%**	**0.01%**	
c11h24	0.011	0.002	0.01%	0.00%	**0.01%**	**0.00%**	
c11h24	0.016	0	0.02%	0.00%	**0.02%**	**0.00%**	
c11h24	0.06	0.005	0.07%	0.00%	**0.06%**	**0.00%**	
c11h24	0.129	0	0.14%	0.00%	**0.13%**	**0.00%**	
c11h24	0.087	0.002	0.10%	0.00%	**0.09%**	**0.00%**	
c11h24	0.013	0.005	0.01%	0.00%	**0.01%**	**0.00%**	
C10H12 TOTAL	0.099	0.037	0.11%	0.03%	**0.10%**	**0.03%**	
c10h12	0.018	0.008	0.02%	0.01%	**0.02%**	**0.01%**	
c10h12	0.023	0.001	0.03%	0.00%	**0.02%**	**0.00%**	
c10h12	0.018	0.01	0.02%	0.01%	**0.02%**	**0.01%**	
c10h12	0.028	0.018	0.03%	0.01%	**0.03%**	**0.01%**	
c10h12	0.012	0	0.01%	0.00%	**0.01%**	**0.00%**	
C11H16 TOTAL	0.306	0.012	0.34%	0.01%	**0.32%**	**0.01%**	
c11h16	0.007	0.001	0.01%	0.00%	**0.01%**	**0.00%**	
c11h16	0.036	0.001	0.04%	0.00%	**0.04%**	**0.00%**	
c11h16	0.01	0.003	0.01%	0.00%	**0.01%**	**0.00%**	
c11h16	0.031	0.002	0.03%	0.00%	**0.03%**	**0.00%**	
c11h16	0.038	0.001	0.04%	0.00%	**0.04%**	**0.00%**	
c11h16	0.119	0.001	0.13%	0.00%	**0.12%**	**0.00%**	
c11h16	0.04	0.001	0.04%	0.00%	**0.04%**	**0.00%**	
c11h16	0.009	0.001	0.01%	0.00%	**0.01%**	**0.00%**	
c11h16	0.003	0.001	0.00%	0.00%	**0.00%**	**0.00%**	
c11h16	0.013	0	0.01%	0.00%	**0.01%**	**0.00%**	
C11H14 TOTAL	0.036	0.001	0.04%	0.00%	**0.04%**	**0.00%**	
c11h14	0.002	0	0.00%	0.00%	**0.00%**	**0.00%**	
c11h14	0.031	0.001	0.03%	0.00%	**0.03%**	**0.00%**	
c11h14	0.003	0	0.00%	0.00%	**0.00%**	**0.00%**	
c12h26	0.068	0	0.08%	0.00%	**0.07%**	**0.00%**	
UNKNOWN TOTAL	0.339	0.079	0.37%	0.06%	**0.35%**	**0.06%**	
Unknown	0.027	0.02	0.03%	0.02%	**0.03%**	**0.01%**	
Unknown	0.042	0.013	0.05%	0.01%	**0.04%**	**0.01%**	
---unknown---	0	0.001	0.00%	0.00%	**0.00%**	**0.00%**	
---unknown---	0	0.003	0.00%	0.00%	**0.00%**	**0.00%**	
---unknown---	0.004	0.001	0.00%	0.00%	**0.00%**	**0.00%**	
Unknown	0	0.001	0.00%	0.00%	**0.00%**	**0.00%**	
---unknown---	0	0.001	0.00%	0.00%	**0.00%**	**0.00%**	
Unknown	0.006	0.001	0.01%	0.00%	**0.01%**	**0.00%**	
---unknown---	0.029	0.01	0.03%	0.01%	**0.03%**	**0.01%**	
Unknown	0.084	0.015	0.09%	0.01%	**0.09%**	**0.01%**	
---unknown---	0.002	0.001	0.00%	0.00%	**0.00%**	**0.00%**	
---unknown---	0.013	0.007	0.01%	0.01%	**0.01%**	**0.00%**	
---unknown---	0.017	0.005	0.02%	0.00%	**0.02%**	**0.00%**	
Unknown	0.115	0	0.13%	0.00%	**0.12%**	**0.00%**	
CO	393.7	510.117					

Table S5: Average Composition of Exhaust Emissions, First 124s of Cold Start (Black 1995-1997)

The Carter carbon bond characterization was determined for all of the measured reactive species that were not included in the MCM. Most of these species were then added to species that did exist in the MCM that had similar or the same reactivity. The list of the species with the Carter break-ups is shown in Table S6. The advantage of this method was to increase the amount of known species to be included in the MCM to 96% of TOG for RFG and to 99% of TOG for E85. The species used in the MCM are summarized in Table S7; the highlighted species are ones that were treated as lumped due to the addition of emission mass to them based on Carter speciation of chemicals not included in the MCM. Including these species makes modeling of secondary species like ozone more accurate without compromising the explicitness of the majority of the species.

The emission data from Table S4 in tonnes/year was then broken up into the individual species according to their % of TOG from the combined Black/Carter emissions profile, for both gasoline and E85, using the TOG for each fuel from the Jacobson study (2007a; 2007b). This assumes the TOG emissions increase by ~22% when using E85 instead of gasoline. The TOG is then split up using the Black/Carter data for gasoline and E85, respectively. An alternate method would have been to split up the gasoline TOG, then use the % change between the E85 data and the gasoline data for each species to determine the E85 emissions. This method was not used for two reasons. First, the gasoline and E85 emissions data from the Black study were taken from two different cars, which makes a percent change in emissions less useful than if the same cars were used. Also, since these data were taken from cold start emissions only and not the full cycle, emissions are higher than during the driving cycle; therefore, it only makes sense to assume the mix of organics is similar for cold start and for full cycle (full cycle includes cold start) and not the amount of emissions.

Exhaust Data from Black; Bold Species are in MCM				Carter Split for CB4											Modified Data	
Compound	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)	Formula	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	UNR	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)
n-dodecane	**0.007**	**0.001**	**C12H26**	**9**										**3**	**0.075**	**0.001**
c12h26	0.068	0	C12H26													
n-undecane	**0.012**	**0.004**	**C11H24**	**8**										**3**	**0.328**	**0.018**
C11H24 TOTAL	0.316	0.014	C11H24													
n-decane	**0.037**	**0.007**	**C10H22**	**8**										**2**	**0.407**	**0.091**
C10H22 TOTAL	0.37	0.084	C10H22													
n-nonane	**0.105**	**0.023**	**C9H20**	**7**										**2**	**1.354**	**0.429**
2,2,5-trimethylhexane	0.551	0.205	C9H20	7										2		
2,3,5-trimethylhexane	0.107	0.04	C9H20	7										2		
2,4-dimethylheptane	0.063	0.018	C9H20	7										2		
2,5-dimethylheptane	0.14	0.04	C9H20	7										2		
2,6-dimethylheptane	0.067	0.019	C9H20	7										2		
3,4-dimethylheptane	0.069	0.017	C9H20	7										2		
3,5-dimethylheptane	0.064	0.021	C9H20	7										2		
1,1,4-trimethylcyclohexane	0.009	0	C9H18	7										2		
3-methyloctane	0.179	0.045	C9H20	7										2		
n-butylcyclopentane	0	0.001	C9H18	7										2		
n-octane	**0.276**	**0.091**	**C8H18**	**7**										**1**	**4.764**	**1.393**
2,3,4-trimethylpentane	1.459	0.4	C8H18	7										1		
2,3-dimethylhexane	0.502	0.149	C8H18	7										1		
2,4-dimethylhexane	0.757	0.196	C8H18	7										1		
2,5-dimethylhexane	0.4	0.124	C8H18	7										1		
3,4-dimethylhexane	0.129	0.046	C8H18	7										1		
2-methylheptane	0.339	0.111	C8H18	7										1		
3-ethylhexane	0.074	0.027	C8H18	7										1		
3-methylheptane	0.383	0.127	C8H18	7										1		
4-methylheptane	0.158	0.055	C8H18	7										1		
cis-1-ethyl-3-methylcyclopentane	0.056	0.016	C8H16	7										1		
trans-1,4-dimethylcyclohexane	0.089	0.022	C8H16	7										1		
trans-1-ethyl-3-methylcyclopentane	0.009	0.002	C8H16	7										1		
isopropylcyclopentane	0.091	0.011	C8H16	7										1		
1,2,3-trimethylcyclopentane	0.017	0.006	C8H16	6.5										1.5		
c,t,c-1,2,3-trimethylcyclopentane	0.025	0.01	C8H16	6.5										1.5		
2-methylhexane	**1.065**	**0.233**	**C7H16**	**6**										**1**	**4.506**	**1.256**
3-methylhexane	**1.146**	**0.251**	**C7H16**	**6**										**1**	**4.587**	**1.274**
n-heptane	**0.668**	**0.165**	**C7H16**	**6**										**1**	**4.109**	**1.188**
2,2,3-trimethylbutane	0.041	0.023	C7H16	6										1		
2,2-dimethylpentane	0.087	0.021	C7H16	6										1		
2,3-dimethylpentane	2.844	0.74	C7H16	6										1		
2,4-dimethylpentane	1.374	0.416	C7H16	6										1		
3,3-dimethylpentane	0.092	0.02	C7H16	6										1		
1,1-dimethylcyclopentane	0.039	0.024	C7H14	6										1		
1-cis-2-dimethylcyclopentane	0.104	0.033	C7H14	6										1		
cis-1,3-dimethylcyclopentane	0.167	0.041	C7H14	6										1		
trans-1,3-dimethylcyclopentane	0.282	0.067	C7H14	6										1		
methylcyclohexane	0.217	0.068	C7H14	6										1		
2,2,3-trimethylpentane	0.008	0.036	C8H18	6										2		
2,2,4-trimethylpentane	5.026	1.561	C8H18	6										2		
1,1,2-trimethylcyclopentane	0.021	0.007	C8H16	6										2		
1,1,3-trimethylcyclopentane	0.02	0.011	C8H16	6										2		
	10.322	3.068														
2,3-dimethylbutane	**0.882**	**0.28**	**C6H14**	**6**											**0.99**	**0.3186**
2-methylpentane	**2.179**	**0.766**	**C6H14**	**6**											**2.287**	**0.8046**
3-methylpentane	**1.252**	**0.353**	**C6H14**	**6**											**1.36**	**0.3916**
N-Hexane	**0.64**	**0.386**	**C6H14**	**6**											**0.748**	**0.4246**
cyclohexane	**0**	**0.023**	**C6H12**	**6**											**0.108**	**0.0616**
methylcyclopentane	0.54	0.193	C6H12	6												
2,2-dimethylbutane	**0.307**	**0.111**	**C6H14**	**5**										**1**	**0.307**	**0.111**
Iso-Pentane	**4.658**	**1.434**	**C5H12**	**5**											**4.694**	**1.4555**
N-pentane	**0.817**	**0.639**	**C5H12**	**5**											**0.853**	**0.6605**
cyclopentane	0.072	0.043	C5H10	5												
1-Hexene	**0.081**	**0.036**	**C6H12**	**4**	**1**										**0.263**	**0.11**
3,3-dimethyl-1-butene	0.015	0.009	C6H12	4	1											
3-methyl-1-pentene	0.167	0.065	C6H12	4	1											
1,2,4-trimethylbenzene	**1.658**	**0.337**	**C9H12**	**4**			**1**								**1.658**	**0.337**
1,3,5-trimethylbenzene	**0.739**	**0.193**	**C9H12**	**4**			**1**								**0.739**	**0.193**
2-Methyl-1-butene	**0.203**	**0.067**	**C5H10**	**4**				**1**							**0.203**	**0.067**
mtbe	**3.06**	**0.922**	**C5H12O**	**4**										**1**	**3.06**	**0.922**
Iso-butane	**0.022**	**0.02**	**C4H10**	**4**											**0.022**	**0.02**
N-Butane	**0.338**	**0.969**	**C4H10**	**4**											**0.338**	**0.969**

Exhaust Data from Black; Bold Species are in MCM				Carter Split for CB4											Modified Data	
Compound (continued)	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)	Formula	PAR	OLE	TOL	XYL	FORM	ALD2	ETH	ISOP	MEOH	ETOH	UNR	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)
2,3-dimethyl-2-butene	**0.028**	**0.009**	**C6H12**	**3.5**				**0.5**	**1**						**0.028**	**0.009**
2-methyl-2-butene	**0.103**	**0.063**	**C5H10**	**3**					**1**						**0.103**	**0.063**
x-valeraldehyde	**0.047**	**0.007**	**C5H10O**	**3**					**1**						**0.047**	**0.007**
3-Methyl-1-Butene	**0.114**	**0.03**	**C5H10**	**3**	**1**										**0.114**	**0.03**
1-Pentene	**0.135**	**0.044**	**C5H10**	**3**	**1**										**0.135**	**0.044**
2-butanone	**0.065**	**0.031**	**C4H8O**	**3**										**1**	**0.065**	**0.031**
2-propanol	**0.312**	**0.04**	**C3H8O**	**3**											**0.312**	**0.04**
acetone	**0.461**	**0.121**	**C3H6O**	**3**											**0.461**	**0.121**
1-Butene	**0**	**0.294**	**C4H8**	**2**	**1**										**0.154**	**0.297**
1-Buten-3-yne	0.126	0	C4H4	2	1											
1,3-Butadiyne	0.028	0.003	C4H2	2	1											
cis-2-hexene	**0.049**	**0.019**	**C6H12**	**2**					**2**						**0.1995**	**0.094**
trans-2-hexene	**0.104**	**0.039**	**C6H12**	**2**					**2**						**0.2545**	**0.114**
4-methyl-cis-2-pentene	0	0.007	C6H12	2					2							
4-methyl-trans-2-pentene	0.104	0.043	C6H12	2					2							
cis-3-methyl-2-pentene	0.035	0.021	C6H12	2					2							
Cis-3-hexene	0.05	0.018	C6H12	2					2							
trans-3-hexene	0.013	0.004	C6H12	2					2							
1-methylcyclopentene	0.037	0.029	C6H10	2					2							
3-methylcyclopentene	0.034	0.014	C6H10	2					2							
4-methylcyclopentene	0.018	0.009	C6H10	2					2							
c6h10	0.01	0.005	C6H10													
	0.301	0.15														
butyraldehyde	**0.063**	**0**	**C4H8O**	**2**					**1**						**0.08**	**0.081**
x-butyraldehyde	**0.044**	**0**	**C4H8O**	**2**					**1**						**0.061**	**0.081**
1-Butyne	0.021	0.105	C4H6	2					1							
2-Butyne	0.013	0.057	C4H6	2					1							
	0.034	0.162														
isopropylbenzene	**0.108**	**0.031**	**C9H12**	**2**		**1**									**0.108**	**0.031**
n-propylbenzene	**0.386**	**0.066**	**C9H12**	**2**		**1**									**0.386**	**0.066**
1,3-dimethyl-5-ethylbenzene	**0.056**	**0.002**	**C10H14**	**2**			**1**								**1.211**	**0.294**
naphthalene	0.135	0.021	C10H8	2			1									
1,2-diethylbenzene	0.055	0.069	C10H18	2			1									
1,3-diethylbenzene	0.15	0.04	C10H18	2			1									
1,2,3,5-tetramethylbenzene	0.025	0.016	C10H14	2			1									
1,2,4,5-tetramethylbenzene	0.095	0.011	C10H14	2			1									
1,2-dimethyl-3-ethylbenzene	0.005	0.006	C10H14	2			1									
1,2-dimethyl-4-ethylbenzene	0.116	0.02	C10H14	2			1									
1,3-dimethyl-2-ethylbenzene	0.051	0.035	C10H14	2			1									
1,3-dimethyl-4-ethylbenzene	0.09	0.02	C10H14	2			1									
1,4-dimethyl-2-ethylbenzene	0.059	0	C10H14	2			1									
1-methyl-2-n-propylbenzene	0.006	0.011	C10H14	2			1									
1-methyl-3-isopropylbenzene	0.038	0.009	C10H14	2			1									
1-methyl-3-n-propylbenzene	0.33	0.034	C10H14	2			1									
Propylene	**3.284**	**1.046**	**C3H6**	**1**	**1**										**3.308**	**1.048**
1,2-Butadiene	0.024	0.002	C4H6	1	1.5											
cis-2-pentene	**0.123**	**0.037**	**C5H10**	**1**					**2**						**0.147**	**0.0545**
trans-2-pentene	**0.235**	**0.064**	**C5H10**	**1**					**2**						**0.259**	**0.0815**
cyclopentene	0.048	0.035	C5H8	1					2							
propionaldehyde	**0.095**	**0.064**	**C3H6O**	**1**					**1**						**0.385**	**0.102**
Methylacetylene	0.29	0.038	C3H5	1					1							
1,2,3-trimethylbenzene	**0.008**	**0.063**	**C9H12**	**1**			**1**								**0.008**	**0.063**
1-methyl-2-ethylbenzene	**0.476**	**0.094**	**C9H12**	**1**			**1**								**0.476**	**0.094**
1-methyl-3-ethylbenzene	**1.474**	**0.298**	**C9H12**	**1**			**1**								**1.474**	**0.298**
1-methyl-4-ethylbenzene	**0.661**	**0.131**	**C9H12**	**1**			**1**								**0.661**	**0.131**
ethylbenzene	**2.412**	**0.731**	**C8H10**	**1**		**1**									**2.412**	**0.731**
benzene	**3.229**	**1.071**	**C6H6**	**1**										**5**	**3.229**	**1.071**
Acetylene	**3.103**	**1.936**	**C2H2**	**1**										**1**	**3.103**	**1.936**
Ethane	**1.26**	**2.255**	**C2H6**	**0.4**										**1.6**	**1.26**	**2.255**
Methane	**5.025**	**15.708**	**CH4**	**0.01**										**0.99**	**5.025**	**15.708**
1,3 Butadiene	**0.507**	**0.067**	**C4H6**		**2**										**0.507**	**0.067**
toluene	**7.688**	**2.273**	**C7H8**			**1**									**7.688**	**2.273**
M&P-Xylene	**5.868**	**1.621**	**C8H10**				**1**								**5.868**	**1.621**
o-xylene	**2.15**	**0.518**	**C8H10**				**1**								**2.15**	**0.518**
formaldehyde	**0.605**	**1.528**	**CH2O**					**1**							**0.605**	**1.528**
Cis-2-Butene	**0.246**	**0.681**	**C4H8**						**2**						**0.246**	**0.681**
Trans-2-Butene	**0.335**	**0.156**	**C4H8**						**2**						**0.335**	**0.156**
acetaldehyde	**0.389**	**12.447**	**C2H4O**						**1**						**0.389**	**12.447**
Ethylene	**4.991**	**10.799**	**C2H4**							**1**					**4.991**	**10.799**
Isoprene	**0.147**	**0.044**	**C5H8**								**1**				**0.147**	**0.044**

Table S6: Species from Black Exhaust Data Added to MCM Species Using Carter’s CB4 Reactivity Ratings (Black 1995-1997; Carter 2008)

Compound	Taurus RFG (ppmC)	Lumina FFV E85 (ppmC)	Taurus RFG (% of TOG)	Lumina FFV E85 (% of TOG)	MCM species name
TOG	95.653	143.518	100%	100%	
TOG in MCM	91.47	142.32	96%	99%	
Methane	5.025	15.708	5.25%	10.94%	CH4
Ethylene (ethene)	4.991	10.799	5.22%	7.52%	C2H4
Ethane	1.26	2.255	1.32%	1.57%	C2H6
Acetylene	3.103	1.936	3.24%	1.35%	C2H2
Propylene	3.308	1.048	3.46%	0.73%	C3H6
Iso-butane	0.022	0.02	0.02%	0.01%	IC4H10
1-Butene	0.154	0.297	0.16%	0.21%	BUT1ENE
Iso-Butylene	4.313	0.548	4.51%	0.38%	MEPROPENE
1,3 Butadiene	0.507	0.067	0.53%	0.05%	C4H6
N-Butane	0.338	0.969	0.35%	0.68%	NC4H10
Trans-2-Butene	0.335	0.156	0.35%	0.11%	TBUT2ENE
Cis-2-Butene	0.246	0.681	0.26%	0.47%	CBUT2ENE
3-Methyl-1-Butene	0.114	0.03	0.12%	0.02%	ME3BUT1ENE
Iso-Pentane	4.694	1.4555	4.91%	1.01%	IC5H12
1-Pentene	0.135	0.044	0.14%	0.03%	PENT1ENE
2-Methyl-1-butene	0.203	0.067	0.21%	0.05%	ME2BUT1ENE
N-pentane	0.853	0.6605	0.89%	0.46%	NC5H12
isoprene	0.147	0.044	0.15%	0.03%	C5H8
trans-2-pentene	0.259	0.0815	0.27%	0.06%	TPENT2ENE
cis-2-pentene	0.147	0.0545	0.15%	0.04%	CPENT2ENE
2-methyl-2-butene	0.103	0.063	0.11%	0.04%	ME2BUT2ENE
2,2-dimethylbutane	0.307	0.111	0.32%	0.08%	M22C4
2,3-dimethylbutane	0.99	0.3186	1.03%	0.22%	M23C4
2-methylpentane	2.287	0.8046	2.39%	0.56%	M2PE
3-methylpentane	1.36	0.3916	1.42%	0.27%	M3PE
1-Hexene	0.263	0.11	0.27%	0.08%	HEX1ENE
N-Hexane	0.748	0.4246	0.78%	0.30%	NC6H14
trans-2-hexene	0.2545	0.114	0.27%	0.08%	THEX2ENE
cis-2-hexene	0.1995	0.094	0.21%	0.07%	CHEX2ENE
2,3-dimethyl-2-butene	0.028	0.009	0.03%	0.01%	DM23BU2ENE
benzene	3.229	1.071	3.38%	0.75%	BENZENE
cyclohexane	0.108	0.0616	0.11%	0.04%	CHEX
2-methylhexane	4.506	1.256	4.71%	0.87%	M2HEX
3-methylhexane	4.587	1.274	4.80%	0.89%	M3HEX
n-heptane	4.109	1.188	4.30%	0.83%	NC7H16
toluene	7.688	2.273	8.04%	1.58%	TOLUENE
n-octane	4.764	1.393	4.98%	0.97%	NC8H18
ethylbenzene	2.412	0.731	2.52%	0.51%	EBENZ
M&P-Xylene	5.868	1.621	6.13%	1.13%	MXYL, PXYL
styrene	0.455	0.079	0.48%	0.06%	STYRENE
o-xylene	2.15	0.518	2.25%	0.36%	OXYL
n-nonane	1.354	0.429	1.42%	0.30%	NC9H20
isopropylbenzene	0.108	0.031	0.11%	0.02%	IPBENZ
n-propylbenzene	0.386	0.066	0.40%	0.05%	PBENZ
1-methyl-3-ethylbenzene	1.474	0.298	1.54%	0.21%	METHTOL
1-methyl-4-ethylbenzene	0.661	0.131	0.69%	0.09%	PETHTOL
1,3,5-trimethylbenzene	0.739	0.193	0.77%	0.13%	TM135B
1-methyl-2-ethylbenzene	0.476	0.094	0.50%	0.07%	OETHTOL
1,2,4-trimethylbenzene	1.658	0.337	1.73%	0.23%	TM124B
n-decane	0.407	0.091	0.43%	0.06%	NC10H22
1,2,3-trimethylbenzene	0.008	0.063	0.01%	0.04%	TM123B
1,3-dimethyl-5-ethylbenzene	1.211	0.294	1.27%	0.20%	DIME35EB
n-undecane	0.328	0.018	0.34%	0.01%	NC11H24
n-dodecane	0.075	0.001	0.08%	0.00%	NC12H26
mtbe	3.06	0.922	3.20%	0.64%	MTBE
methanol	0.229	6.684	0.24%	4.66%	CH3OH
ethanol	0.026	67.309	0.03%	46.90%	C2H5OH
2-propanol	0.312	0.04	0.33%	0.03%	IPROPOL
formaldehyde	0.605	1.528	0.63%	1.06%	HCHO
acetaldehyde	0.389	12.447	0.41%	8.67%	CH3CHO
acetone	0.461	0.121	0.48%	0.08%	CH3COCH3
propionaldehyde	0.385	0.102	0.40%	0.07%	C2H5CHO
butyraldehyde	0.08	0.081	0.08%	0.06%	C3H7CHO
benzaldehyde	0.255	0.088	0.27%	0.06%	BENZAL
x-butyraldehyde	0.061	0.081	0.06%	0.06%	IPRCHO
x-valeraldehyde	0.047	0.007	0.05%	0.00%	C4H9CHO
2-butanone	0.065	0.031	0.07%	0.02%	MEK
dimethyl ether	0.041	0.007	0.04%	0.00%	CH3OCH3
1,3-diethyl 5-methylbenzene	0.306	0.012	0.32%	0.01%	DIET35TOL

Table S7: Summary of Species from Exhaust Emissions from Black Data for MCM

Note: Highlighted Species Include Species not in the MCM (Black 1995-1997; Carter 2008)

The emissions we have discussed so far were all measured under standard conditions (24 to 25 C). Two studies have measured emissions under both warm (22 C) and cold (-7 C) ambient temperatures (Whitney and Fernandez 2007; Westerholm et al. 2008). Westerholm et al. (2008) measured the emissions from two different flex-fuel vehicles (Saab and Volvo), for gasoline (E5, 5% ethanol, 95% gasoline), E70 (70% ethanol, 30% gasoline) and E85. Whitney and Fernandez. (2007) measured the emissions from three different flex-fuel vehicles (Chevrolet, Lincoln, and Dodge) for gasoline (E0), E70, and E85. The vehicles differed in type and fuel economy, as shown in Table S8. However, much of the emissions results for both warm and cold ambient temperatures were similar between the different vehicles.

					Fuel Economy (mpg)*	
Study	**Vehicles**	**Year**	**Type**	**Engine type**	**E85**	**Gasoline**
Westerholm (2008)	Saab 9-5 Biopower	2005	Wagon	L4	19	25
Westerholm (2008)	Volvo V50 1.8 F	2005	Wagon	L4		26.5
Whitney (2007)	Chevrolet Silverado	2007	Pickup Truck	5.3L V8	12	16
Whitney (2007)	Lincoln Town Car	2006	Car	4.6L V8	13	18
Whitney (2007)	Dodge Stratus	2006	Car	2.7L V6	16	21

Table S8: Vehicles Used for Emissions Studies of Ethanol Fuels at Warm and cold Temperatures.

NOTE: Fuel economy measurements are from (West et al. 2007) for the Saab, http://www.whatgreencar.com/view-car/21310/volvo-v50-1_8F_Flexifuel_2009 for the Volvo, and www.fueleconomy.gov for the Chevrolet, Lincoln, and Dodge

The emissions results are shown in Table S10 and Table S9. The actual emissions amounts differ, but the % change from gasoline to ethanol fuel are generally in the same direction and of similar magnitude. Hydrocarbons, formaldehyde, acetaldehyde, and ethanol all increased from gasoline to E70 and from gasoline to E85 for both warm and cold ambient temperatures with only a couple of exceptions (Whitney and Fernandez 2007; Westerholm et al. 2008). Hydrocarbons decreased for the Chevrolet Silverado from gasoline to E85, for the Lincoln Town Car from gasoline to E70 and for the Volvo V50 from gasoline to E85, all at the warm ambient temperature (Table S9). Another exception was the decrease in formaldehyde emission from the Lincoln Town Car for E70 at 22 C. The results for 1,3-butadiene and benzene were more mixed. For -7 C, 1,3-butadiene increased for the Chevrolet and the Volvo by 20% to 59%. It decreased for the Lincoln and Dodge by -14% and -7%, respectively (Table S10). 1,3-Butadiene decreased for all vehicles except the Volvo at 22 C by -71% to -43%. It increased by only 8% for the Volvo. At -7 C, benzene decreased for E70 for the Chevrolet, the Lincoln, and the Volvo. Surprisingly, it actually increased for E70 for the Dodge and for E85 for the Volvo (Table S10). The benzene should only be present in the gasoline portion of the fuel, so any increase in benzene emissions when switching from gasoline to ethanol fuels is unexpected. The warm temperature emissions of benzene decreased for all vehicles from gasoline to ethanol fuel, as expected (Table S9).

For the application of our model, we use the Volvo emissions data set to examine how colder ambient temperatures might impact air pollution. The Saab and Volvo vehicles were the only ones measured at -7C for E85, and the Saab has a lot of missing values in its data set. The Volvo is the most complete data set and therefore is best suited for use in our study. The complete data set for the Saab and the Volvo is shown in Table S11 (Westerholm et al. 2008).

Emissions (g/km)	Whitney et al. (2007)									Westerholm et al. (2008)									
Temp = -7C	2007 Chevrolet Silverado			2006 Lincoln Town Car			2006 Dodge Stratus			2005 Saab 9-5 Biopower					2005 Volvo V50				
Species	Gasoline (E0)	E70	% Change	Gasoline (E0)	E70	% Change	Gasoline (E0)	E70	% Change	Gasoline (E5)	E70	% Change	E85	% Change	Gasoline (E5)	E70	% Change	E85	% Change
HC*										0.30	1.20	300%	1.77	490%	0.43	1.14	165%	1.25	191%
NMHC**	0.30	0.58	96%	0.37	0.76	107%	0.26	0.77	195%										
Formaldehyde	0.00042	0.0017	300%	0.00039	0.00081	108%	0.000093	m.v.		m.v.	m.v.		0.0091		0.0008	0.0036	350%	0.0032	300%
Acetaldehyde	0.00031	0.026	8300%	0.00031	0.025	8100%	m.v.	m.v.		m.v.	m.v.		0.1229		0.0066	0.12	1702%	0.093	1314%
Ethanol	0	0.286		0	0.572		m.v.	m.v.		m.v.	m.v.		1.441		0.024	1.21	4929%	1.22	4996%
1,3-Butadiene	0.00057	0.00068	20%	0.00045	0.00039	-14%	0.00046	0.00043	-7%	m.v.	m.v.		0.0021		0.00078	0.00098	26%	0.0012	59%
Benzene	0.0081	0.0056	-31%	0.011	0.0078	-31%	0.0061	0.0071	18%	m.v.	m.v.		0.016		0.013	0.01	-19%	0.014	9%

Table S10: Vehicle Emissions Comparison for Cold Ambient Temperatures (T = -7C) *(37,38)*

NOTE: *HC = Hydrocarbons calculated based on average gasoline carbon/hydrogen ratio and was not adjusted for ethanol fuels. **NMHC = non-methane hydrocarbons were corrected for ethanol.

Emissions (g/km)	Whitney et al. (2007)															Westerholm et al. (2008)					
Temp = 22C	2007 Chevrolet Silverado					2006 Lincoln Town Car					2006 Dodge Stratus					2005 Saab 9-5 Biopower			2005 Volvo V50		
Species	Gasoline (E0)	E70	% Change	E85	% Change	Gasoline (E0)	E70	% Change	E85	% Change	Gasoline (E0)	E70	% Change	E85	% Change	Gasoline (E5)	E85	% Change	Gasoline (E5)	E85	% Change
HC*																0.06	0.08	33%	0.07	0.05	-29%
NMHC**	0.027	0.036	31%	0.023	-14%	0.026	0.024	-9%	0.033	26%	0.022	0.026	18%	0.028	29%						
Formaldehyde	0.00022	0.00041	83%	0.00055	147%	0.00015	0.00012	-21%	0.0003	104%	0.000205	m.v.		m.v.		0.0007	0.0021	200%	0.0006	0.0016	167%
Acetaldehyde	0.000093	0.0031	3233%	0.0025	2533%	0.000062	0.0019	2900%	0.004	6400%	0.000062	m.v.		m.v.		0.0012	0.018	1367%	0.0013	0.0103	692%
Ethanol	0	0.01		0.016		0	0.0070		0.011		0	m.v.		m.v.		0.006	0.078	1200%	0.001	0.068	6700%
1,3-Butadiene	0.000065	0.00003	-54%	0.000021	-67%	0.000048	0.000014	-71%	0.000016	-67%	0.000072	0.000041	-43%	0.000025	-65%	0.00051	0.0002	-61%	0.00037	0.0004	8%
Benzene	0.00011	0.0001	-9%	0.000043	-59%	0.00014	0.000062	-56%	0.00004	-71%	0.00012	m.v.		m.v.		0.0022	0.001	-55%	0.0023	0.0002	-91%

Table S9: Vehicle Emissions Comparison for Warm Ambient Temperatures (T = 22C) *(37,38)*

NOTE: *HC = Hydrocarbons calculated based on average gasoline carbon/hydrogen ratio and was not adjusted for ethanol fuels. **NMHC = non-methane hydrocarbons were corrected for ethanol.

	NEDC (22 C) (g/km)		NEDC (-7 C) (g/km)		From 22 C to -7 C		From E5 to E85	
	E5	E85	E5	E85	% Change E5	% Change E85	% Change 22 C	% Change -7 C
Saab - CO	0.58	1.02	1.73	4.45	198%	336%	76%	157%
Volvo - CO	0.89	0.23	4.61	6.07	418%	2539%	-74%	32%
Avg CO					**308%**	**1438%**	**1%**	**94%**
Saab - HC*	0.06	0.08	0.3	1.77	400%	2113%	33%	490%
Volvo - HC*	0.07	0.05	0.43	1.25	514%	2400%	-29%	191%
Avg HC					**457%**	**2256%**	**2%**	**340%**
Saab - NOx	0.02	0.01	0.7	0.078	3400%	680%	-50%	-89%
Volvo - NOx	0.04	0.03	0.034	0.05	-15%	67%	-25%	47%
Avg NOx					**1693%**	**373%**	**-38%**	**-21%**
Saab - PM	0.0001	0.0002	0.004	0.0047	3900%	2250%	100%	18%
Volvo - PM	0.0004	0.0002	0.0031	0.0046	675%	2200%	-50%	48%
Avg PM					**2288%**	**2225%**	**25%**	**33%**
Saab - CH4	0.008	0.019	0.022	0.13	175%	584%	138%	491%
Volvo - CH4	0.005	0.008	0.02	0.087	300%	988%	60%	335%
Avg CH4					**238%**	**786%**	**99%**	**413%**
Saab - HCHO	0.0007	0.0021		0.0091		333%	200%	
Volvo - HCHO	0.0006	0.0016	0.0008	0.0032	33%	100%	167%	300%
Avg HCHO					**33%**	**217%**	**183%**	**300%**
Saab - CH3CHO	0.0012	0.0176		0.1229		598%	1367%	
Volvo - CH3CHO	0.0013	0.0103	0.0066	0.0933	408%	806%	692%	1314%
Avg CH3CHO					**408%**	**702%**	**1029%**	**1314%**
Saab - C2H5OH	0.006	0.078		1.441		1747%	1200%	
Volvo - C2H5OH	0.001	0.068	0.024	1.223	2300%	1699%	6700%	4996%
Avg C2H5OH					**2300%**	**1723%**	**3950%**	**4996%**
Saab - NH3	0	0		0				
Volvo - NH3	0	0	0.018	0.017				-6%
Avg NH3								**-6%**
Saab - ethene	0.004	0.01		0.038		280%	150%	
Volvo - ethene	0.004	0.003	0.017	0.056	325%	1767%	-25%	229%
Avg ethene					**325%**	**1023%**	**63%**	**229%**
Saab - propene	0.0028	0.0012		0.0138		1050%	-57%	
Volvo - propene	0.0038	0.0007	0.0132	0.0159	247%	2171%	-82%	20%
Avg propene					**247%**	**1611%**	**-69%**	**20%**
Saab - 1,3 butadiene	0.00051	0.0002		0.00214		970%	-61%	
Volvo - 1,3 butadiene	0.00037	0.0004	0.00078	0.00124	111%		8%	59%
Avg 1,3 butadiene					**111%**	**970%**	**-26%**	**59%**
Saab - benzene	0.0022	0.001		0.0159		1490%	-55%	
Volvo - benzene	0.0023	0.0002	0.0126	0.0137	448%		-91%	9%
Avg benzene					**448%**	**1490%**	**-73%**	**9%**
Saab - toluene	0.006	0.003		0.056		1767%	-50%	
Volvo - toluene	0.007	0.001	0.056	0.052	700%	5100%	-86%	-7%
Avg toluene					**700%**	**3433%**	**-68%**	**-7%**

Table S11: The Tailpipe Emissions for the Saab 9-5 Biopower and the Volvo V50 flex-fuel vehicle for Ambient Temperatures 22 C (71.6 F) and -7 C (19.4 F) (Westerholm et al. 2008)

Note: *HC - Hydrocarbon data was calculated based on average gasoline carbon/hydrogen ratio and was not adjusted for ethanol fuels.

To determine the emissions data at -7 C, we first assumed the current data we have represents the emissions data at 22 C, which is a good assumption since most of the data were taken at an ambient temperature of around 24 C. We then use these data to determine the % change from gasoline (E5) at 22 C to gasoline (E5) at -7 C for the Volvo, as shown in Table S11. This % change was then applied to the gasoline emissions data for each species measured by Westerholm et al (2008). The remaining hydrocarbon emissions were calculated by breaking up the remaining % change in total hydrocarbons (not including alcohols) over the rest of the species. For example, for gasoline (E5), the following species were measured explicitly by Westerholm et al. (2008) and their % change from 22 C to -7 C can be applied directly: carbon monoxide (CO), methane, formaldehyde, acetaldehyde, ethanol, ethane, propene, 1,3-butadiene, benzene, and toluene. For CO, the Volvo % change of gasoline (E5) emissions from 22 C to -7 C was 418%. To calculate the new tonnes/year for CO emissions for -7 C in the LA area, the emissions from Jacobson (2007a) for CO = 782,000 tonnes/year was multiplied by the % change, 418%, and added to the emissions from Jacobson (2007a), to give 4,050,584 tonnes/year of CO at -7 C ambient temperature. To determine the % change for the hydrocarbons that were not explicitly measured by Westerholm et al. (2008), the total hydrocarbons minus the alcohols were summed for the Black/Carter emissions data, giving 85,732 tonnes/year of hydrocarbons for gasoline. The Volvo % change, 514%, of the total hydrocarbons from 22 C to -7 C from Westerholm et al. (2008) was then applied to this number, to give 526,639 tonnes/year of hydrocarbons at -7 C. The sum of the explicit hydrocarbons (methane, formaldehyde, acetaldehyde, ethane, propene, 1,3-butadiene, benzene, and toluene, which was 24,196 tonnes/year for 22 C and 127,689 tonnes/year for -7 C) was then subtracted from the total hydrocarbons. The remaining hydrocarbons were 61,536 tonnes/year for 22 C and 398,950 tonnes/year for -7 C. The % change for these remaining hydrocarbons was then calculated by dividing 398,950 by 61,536 and subtracting 1 to give 548%. This % change was then applied to all of the remaining hydrocarbons. Since methanol and 2-propanol, both alcohols, were not included in the explicit measurements and not included in the total hydrocarbons, their emissions were assumed to stay the same when the temperature decreased from 22 C to -7 C. This is a conservative assumption because the alcohol emissions likely increased substantially under colder conditions, similar to the increase seen for ethanol (2300%).

Once the emissions were known for gasoline at -7 C, the % change between gasoline and E85 at -7 C for Volvo could be used to calculate the E85 emissions at -7 C for all of the explicitly measured species. A similar system as described above was used to calculate the change in emissions for the remaining hydrocarbons. Again, methanol and 2-propanol emissions were assumed to remain the same when the temperature changed from 22 C to -7 C for E85 because there was no measured data for these alcohols. The results are shown in Table S12. The total % changes from gasoline to E85 for the different scenarios are summarized in Table S13, where a positive % means there is an increase in the emissions of that species when using E85 instead of gasoline.

	Gasoline (tonnes/yr)		E85 (tonnes/year)	
Species Name	24 C Emissions Set	-7 C Emissions Set	24 C Emissions Set	-7 C Emissions Set
CO	782,000	4,050,584	821,100	5,333,416
NOx	68,900	58,565	48,230	86,125
NO2	62,010	52,709	43,407	77,513
NO	6,890	5,857	4,823	8,613
Methane	4,723	18,893	12,010	82,184
Ethylene (ethene)	4,691	19,938	8,256	65,678
Ethane	1,184	7,678	1,724	122,358
Acetylene	2,917	18,909	1,480	105,049
Propylene (propene)	3,109	10,801	801	13,010
Iso-butane	21	134	15	1,085
1-Butene	145	938	227	16,115
Iso-Butylene	4,054	26,283	419	29,735
1,3 Butadiene	477	1,005	51	1,597
N-Butane	318	2,060	741	52,579
Trans-2-Butene	315	2,041	119	8,465
Cis-2-Butene	231	1,499	521	36,952
3-Methyl-1-Butene	107	695	23	1,628
Iso-Pentane	4,412	28,605	1,113	78,976
1-Pentene	127	823	34	2,387
2-Methyl-1-butene	191	1,237	51	3,635
N-pentane	802	5,198	505	35,839
isoprene	138	896	34	2,387
trans-2-pentene	243	1,578	62	4,422
cis-2-pentene	138	896	42	2,957
2-methyl-2-butene	97	628	48	3,418
2,2-dimethylbutane	289	1,871	85	6,023
2,3-dimethylbutane	931	6,033	244	17,287
2-methylpentane	2,150	13,937	615	43,658
3-methylpentane	1,278	8,288	299	21,248
1-Hexene	247	1,603	84	5,969
N-Hexane	703	4,558	325	23,039
trans-2-hexene	239	1,551	87	6,186
cis-2-hexene	188	1,216	72	5,101
2,3-dimethyl-2-butene	26	171	7	488
benzene	3,035	16,627	819	18,079
cyclohexane	102	658	47	3,342
2-methylhexane	4,235	27,457	960	68,133
3-methylhexane	4,311	27,951	974	69,110
n-heptane	3,862	25,038	908	64,444
toluene	7,226	57,811	1,738	53,681
n-octane	4,478	29,031	1,065	75,585
ethylbenzene	2,267	14,699	559	39,665
M&P-Xylene	5,516	35,759	1,239	87,957
styrene	428	2,773	60	4,287
o-xylene	2,021	13,102	396	28,107
n-nonane	1,273	8,251	328	23,278
isopropylbenzene	102	658	24	1,682
n-propylbenzene	363	2,352	50	3,581
1-methyl-3-ethylbenzene	1,385	8,982	228	16,170
1-methyl-4-ethylbenzene	621	4,028	100	7,108
1,3,5-trimethylbenzene	695	4,503	148	10,472
1-methyl-2-ethylbenzene	447	2,901	72	5,101
1,2,4-trimethylbenzene	1,558	10,104	258	18,286
n-decane	383	2,480	70	4,938
1,2,3-trimethylbenzene	8	49	48	3,418
1,3-dimethyl-5-ethylbenzene	1,138	7,380	225	15,953
n-undecane	308	1,999	14	977
n-dodecane	70	457	1	54
mtbe	2,876	18,647	705	50,028
methanol	215	215	5,110	5,110
ethanol	24	587	51,462	29,889
2-propanol	293	293	31	31
formaldehyde	569	758	1,168	3,033
acetaldehyde	366	1,856	9,516	26,242
acetone	433	2,809	93	6,566
propionaldehyde	362	2,346	78	5,535
butyraldehyde	75	488	62	4,395
benzaldehyde	240	1,554	67	4,775
x-butyraldehyde	57	372	62	4,395
x-valeraldehyde	44	286	5	380
2-butanone	61	396	24	1,682
dimethyl ether	39	250	5	380
1,3-diethyl 5-methylbenzene	288	1,865	9	651

Table S12: The Total Emissions for Gasoline and E85 for the SCAB in 2020 for 24 C and -7 C Emissions Sets

Note: 24 C Emissions set: Jacobson (2007a), Black (1995-1997) and Carter (2008); -7 C Emissions Set: Jacobson (2007a), and Westerholm et al. (2008); The alcohol emissions do not change except for ethanol because the alcohols were not measured in the Westerholm et al. data (2008)

Species	MCM Species	Jacobson (2007)	24 C Emissions Set	-7 C Emissions Set
CO	CO	5%		32%
CO2	CO2			
NOx		-30%		47%
Methane	CH4	43%	154%	335%
Ethylene (ethene)	C2H4	-17%	76%	229%
Ethane	C2H6	0%	46%	1494%
Acetylene	C2H2		-49%	456%
Propylene (propene)	C3H6	-65%	-74%	20%
Iso-butane	IC4H10		-26%	709%
1-Butene	BUT1ENE		57%	1617%
Iso-Butylene	MEPROPENE		-90%	13%
1,3 Butadiene	C4H6	-10%	-89%	59%
N-Butane	NC4H10		133%	2453%
Trans-2-Butene	TBUT2ENE		-62%	315%
Cis-2-Butene	CBUT2ENE		125%	2365%
3-Methyl-1-Butene	ME3BUT1ENE		-79%	134%
Iso-Pentane	IC5H12		-75%	176%
1-Pentene	PENT1ENE		-73%	190%
2-Methyl-1-butene	ME2BUT1ENE		-73%	194%
N-pentane	NC5H12		-37%	589%
C5H8 TOTAL	C5H8	-80%	-76%	167%
trans-2-pentene	TPENT2ENE		-74%	180%
cis-2-pentene	CPENT2ENE		-70%	230%
2-methyl-2-butene	ME2BUT2ENE		-50%	445%
2,2-dimethylbutane	M22C4		-71%	222%
2,3-dimethylbutane	M23C4		-74%	187%
2-methylpentane	M2PE		-71%	213%
3-methylpentane	M3PE		-77%	156%
1-Hexene	HEX1ENE		-66%	272%
N-Hexane	NC6H14		-54%	405%
trans-2-hexene	THEX2ENE		-64%	299%
cis-2-hexene	CHEX2ENE		-62%	320%
2,3-dimethyl-2-butene	DM23BU2ENE		-74%	186%
benzene	BENZENE	-79%	-73%	9%
cyclohexane	CHEX		-54%	408%
2-methylhexane	M2HEX		-77%	148%
3-methylhexane	M3HEX		-77%	147%
n-heptane	NC7H16		-76%	157%
toluene	TOLUENE	-80%	-76%	-7%
n-octane	NC8H18		-76%	160%
ethylbenzene	EBENZ		-75%	170%
M&P-Xylene	MXYL, PXYL	-80%	-78%	146%
styrene	STYRENE		-86%	55%
o-xylene	OXYL	-80%	-80%	115%
n-nonane	NC9H20		-74%	182%
isopropylbenzene	IPBENZ		-77%	156%
n-propylbenzene	PBENZ		-86%	52%
1-methyl-3-ethylbenzene	METHTOL		-84%	80%
1-methyl-4-ethylbenzene	PETHTOL		-84%	76%
1,3,5-trimethylbenzene	TM135B		-79%	133%
1-methyl-2-ethylbenzene	OETHTOL		-84%	76%
1,2,4-trimethylbenzene	TM124B		-83%	81%
n-decane	NC10H22		-82%	99%
1,2,3-trimethylbenzene	TM123B		541%	6912%
1,3-dimethyl-5-ethylbenzene	DIME35EB		-80%	116%
n-undecane	NC11H24		-96%	-51%
n-dodecane	NC12H26		-99%	-88%
mtbe	MTBE		-75%	168%
methanol	CH3OH		2274%	2274%
ethanol	C2H5OH	increase	210475%	4996%
2-propanol	IPROPOL		-90%	-90%
formaldehyde	HCHO	60%	105%	300%
acetaldehyde	CH3CHO	2000%	2503%	1314%
acetone	CH3COCH3	0%	-79%	134%
propionaldehyde	C2H5CHO		-78%	136%
butyraldehyde	C3H7CHO		-18%	802%
benzaldehyde	BENZAL		-72%	207%
x-butyraldehyde	IPRCHO		8%	1082%
x-valeraldehyde	C4H9CHO		-88%	33%
2-butanone	MEK		-61%	325%
dimethyl ether	CH3OCH3		-86%	52%
1,3-diethyl 5-methylbenzene	DIET35TOL		-97%	-65%
Propane		-65%		
Paraffin bond group (PAR)		-80%		
Olefin bond group (OLE)		-17%		
Higher Aldehydes		-60%		

Table S13: % Change in Emissions from Gasoline to E85 for Each Species

Now we have two sets of emissions for gasoline and E85 – at 24 C and at -7 C. These emissions sets were then investigated over a range of temperatures – above zero degrees C for the 24 C emissions set, and below zero degrees C for the -7 C emissions set. Since the below zero temperatures would be more likely to occur in the winter, the solar profile for the model was modified for the model runs at low temperature. The January solar profile for the Los Angeles area was chosen as the model solar profile for these low temperature emissions. Even though the Los Angeles area does not regularly get down to these low temperatures, even in winter, the results will demonstrate how the air pollution in cold areas with sparse vegetation and large vehicle fleets is likely to change when gasoline is replaced with E85-powered flex-fuel vehicles. The sunrise was changed from 6 am to 7 am and the sunset from 6 pm to 5 pm, shortening the solar radiation over the day, as shown in Figure S11. The insolation is also decreased in the winter – in addition to the shortened day. The insolation in the Los Angeles area on a clear day in the summer is about 980 W/m^2. The insolation for a clear day in January is about 630 W/m^2, only about 64% of a clear summer day. Also, clouds are more prevalent in the winter in L.A. To account for this, the max photolysis rates were decreased by half for the winter model run, to account for lower insolation and cloud cover. This is represented by the lower insolation in Figure S11. Not unexpectedly, reducing the insolation dramatically decreases the amount of ozone produced, especially for E85.

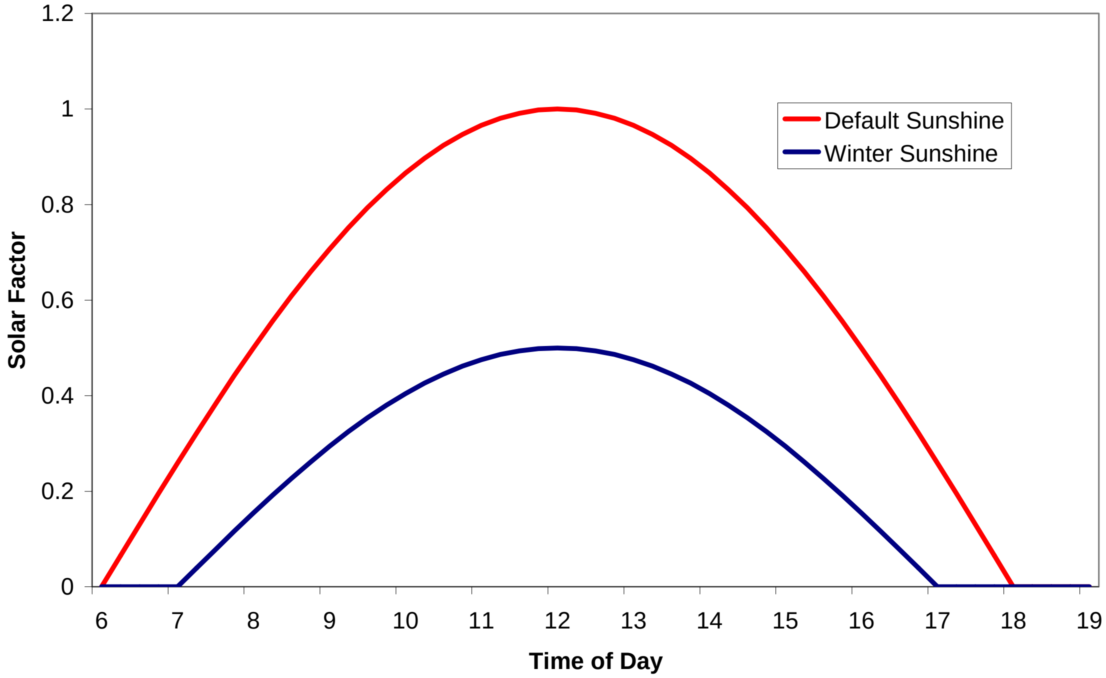

Figure S11: Representation of the Solar Intensity for 24 C Emissions (Default, or Summer, Sunshine) and -7 C Emissions (Winter Sunshine)

The ambient temperature followed a sine profile in the daytime, increasing in the morning and decreasing in the afternoon, and was constant at night. This profile was chosen based on temperature data from CARB for the SCAB (CARB 2008). The temperature was measured for many different cities/towns in the SCAB – so a representative profile was chosen by comparing the profile of all of these different areas for a day in July, shown in Figure S12, and a day in August, shown in Figure S13. A few days in February were also examined to make sure the profile is similar in winter even though the temperatures are cooler, as shown in Figure S14.

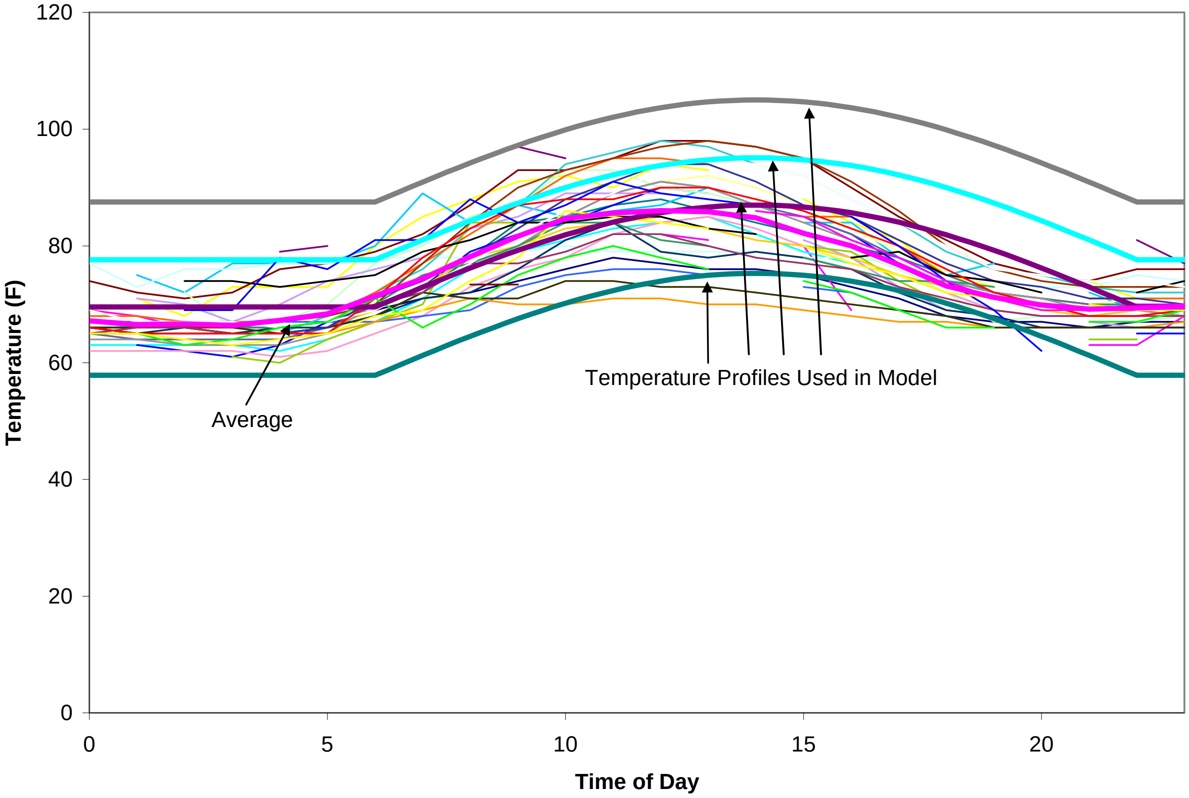

Figure S12: July 10th, 2008 Temperature Profiles for Cities in the SCAB with the Model Temperature Profiles in Bold (CARB 2008)

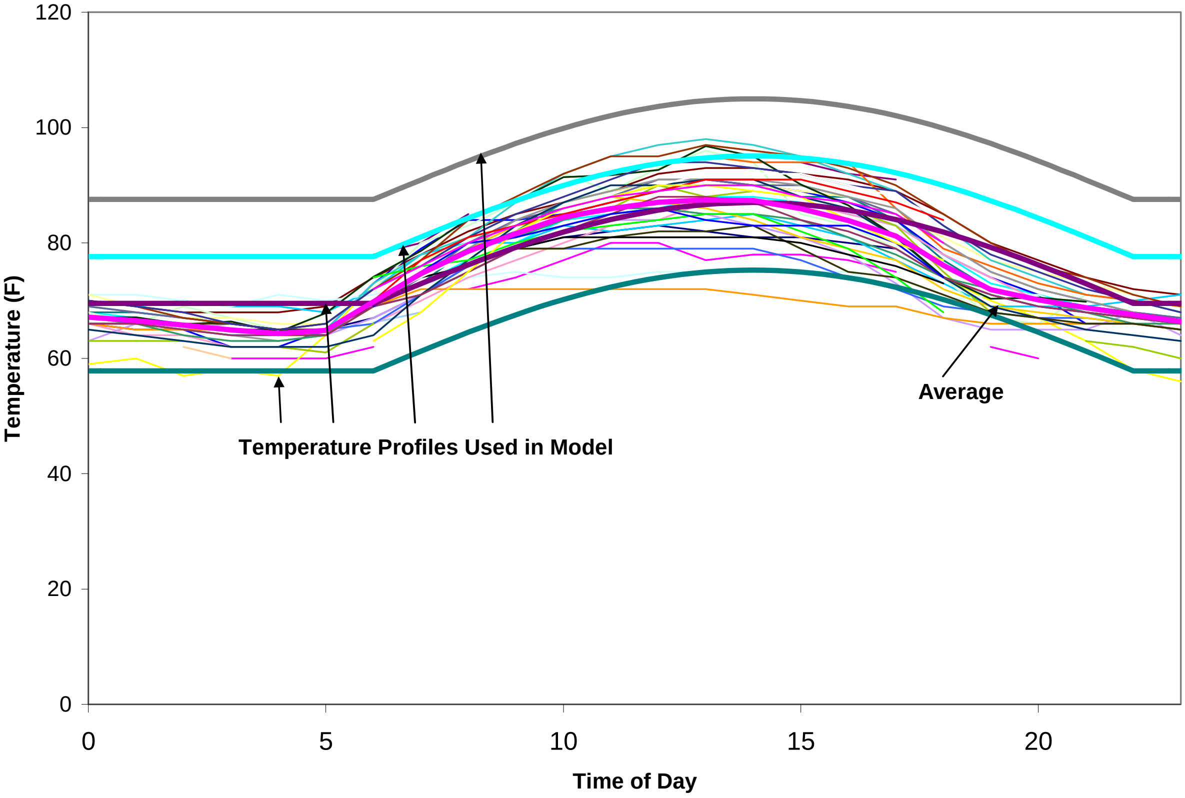

Figure S13: August 10th, 2008 Temperature Profiles for Cities in the SCAB with the Model Temperature Profiles in Bold (CARB 2008)

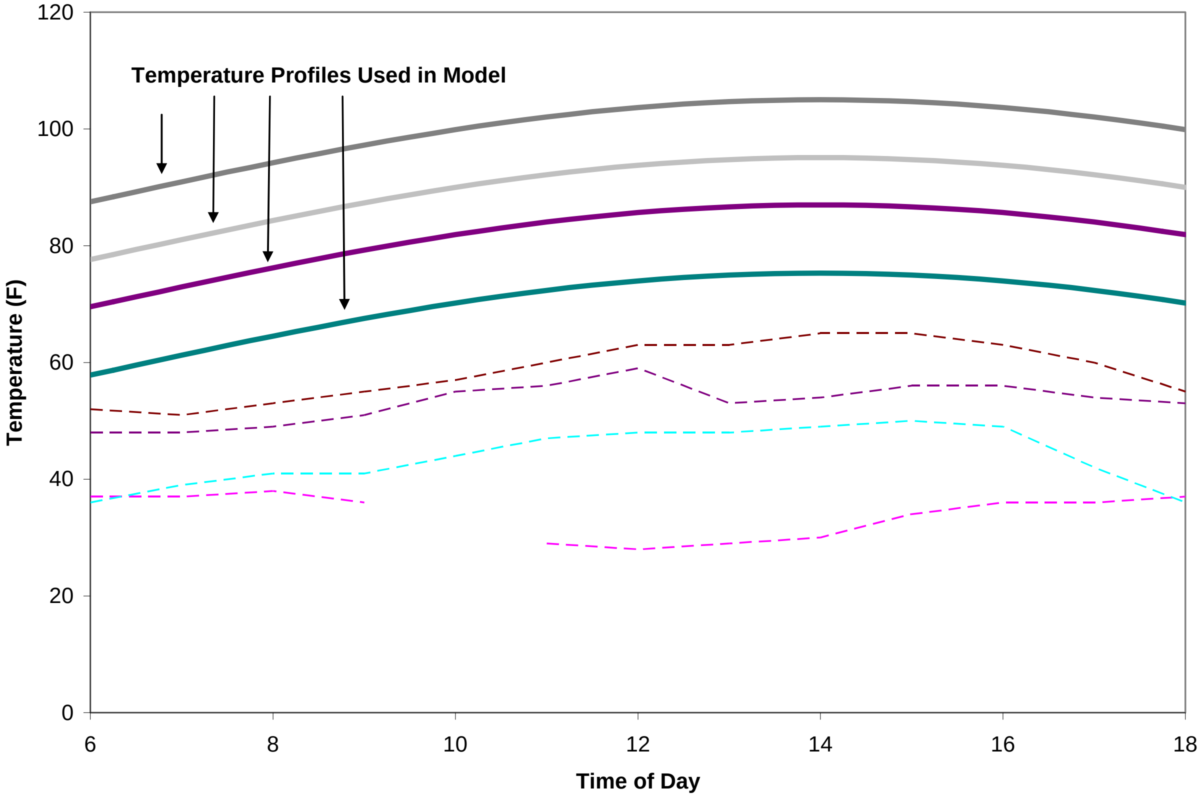

Figure S14: February 14th and 15th, 2008 Temperature Profiles for Cities in the SCAB with the Model Temperature Profiles in Bold (CARB 2008)

The temperature profile was calculated as follows. First, an average temperature profile was calculated from the temperature data for a day in July (Figure S12) and a day in August (Figure S13). The peak of this average temperature profile was 2 pm, so this was chosen as the peak for all of the temperature profiles used in the SCAB modeling study ($t_{peak} = 28{,}000$ s). A factor was chosen by trying to match the average profile (9.705555). Therefore, the temperature profile for the SCAB modeling was:

$$T = T_i + 9.705555*\sin((t*(pi/2))/28800)$$

To look at the sensitivity of the system to temperature, the initial temperature was changed to target different peak temperatures (35 C, 41 C, etc) as shown in Figure S15. The temperature profile will be referred to by its peak temperature in this report.

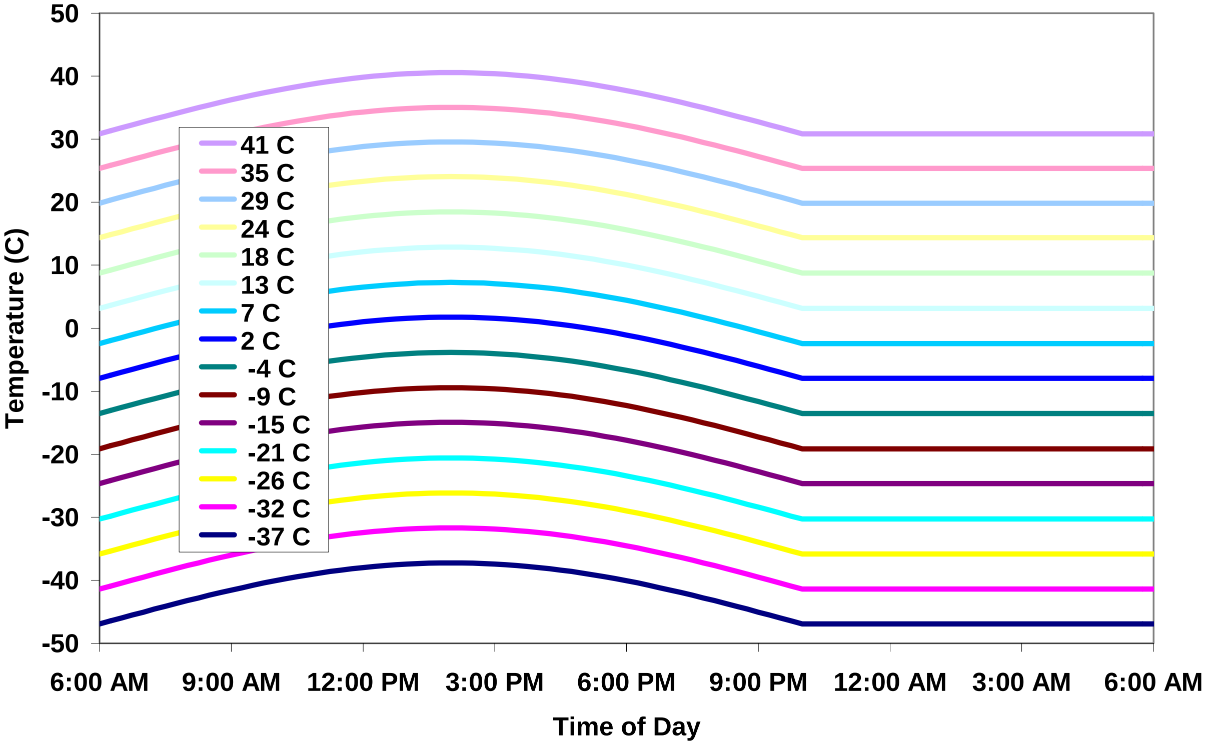

Figure S15: Temperature Profiles Used in the Model for Each Day, Labeled by their Peak Temperature

The box model was sized to match the SCAB to make these emissions appropriate. The area of the SCAB is 6,745 mi^2 and is shown in Figure S16 (AQMD 2008). The area used for this box model was 1.5 degrees latitude by 1.1 degrees longitude, which is 6,751 mi^2, approximately the same as the SCAB. The baseline height of the box was 500 m. The sensitivity of the results to the mixing height was investigated by examining the results for 300 m and 1 km.

Figure S16: Map of the South Coast Air Basin (SCAB) (AQMD 2008)

The next step was to determine the emission rate for gasoline and E85 for the SCAB for each day. The vehicle emissions profile, shown in Figure S17 for a few species, describes what might happen on a typical weekday in Los Angeles. The profile is based on the diurnal profile for urban vehicles from the Emissions Modeling Clearinghouse Temporal Allocation by the U.S. Environmental Protection Agency (USEPA 2000).

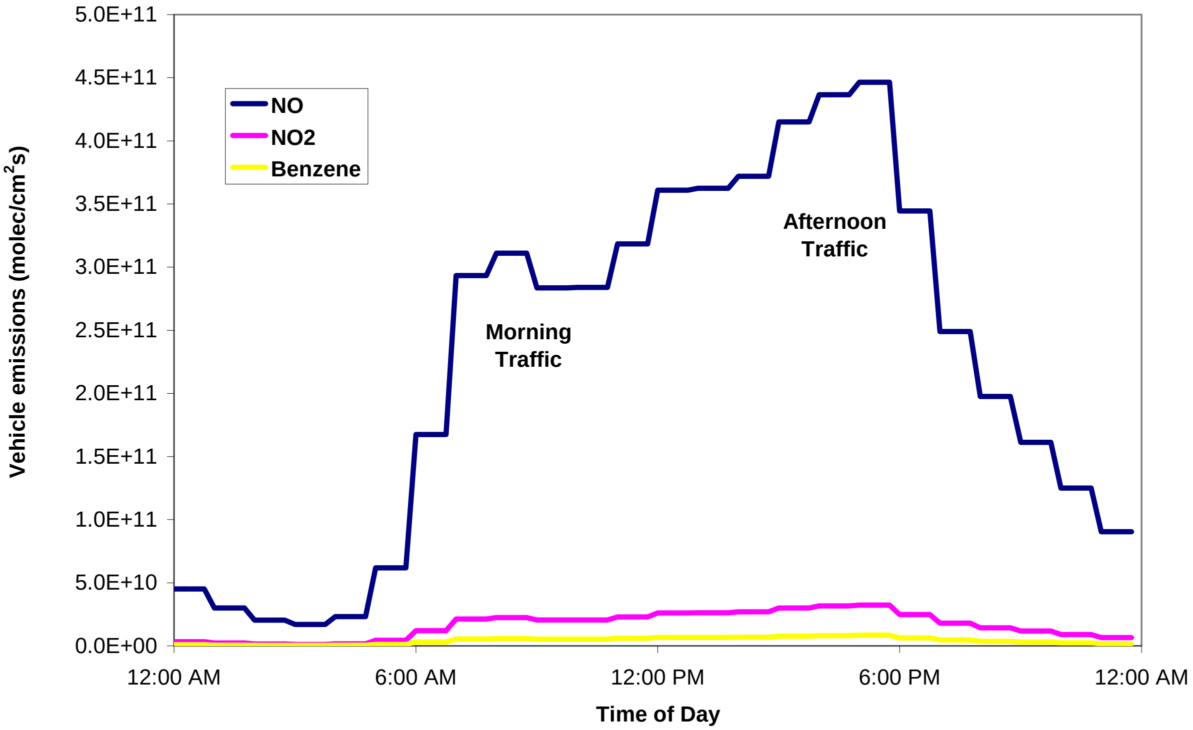

Figure S17: The Vehicle Emissions Profile for All Emitted Species, Shown for Three Example Species

In addition to vehicle emissions, the model needs the background emissions in order to more accurately calculate ozone levels. The background emissions were the same for the gasoline scenario and the E85 scenario and are listed in Table S14 (Jacobson 2007a; Jacobson 2007b). The background emissions include point, fugitive, area, non-road non-gasoline, and on-road non-gasoline emissions. The background emissions are from Jacobson (2007a; 2007b) and were used in an ACBM, so some of the groups of species/bonds (PAR, OLE, ALD2) had to be split up and assigned to individual species in order to fit the MCM. This was done again using the Carter method for breaking up species according to their carbon bond – only this time it was done in the reverse (Carter 2008). The species that were used in place of these carbon bond categories were chosen by three criteria: 1) they did not already have background emissions listed; 2) they existed in the MCM; and 3) they were the simplest species that fit the requirements. For the Olefin bond group (OLE), 1-butene (PAR = 2, OLE =1) was used to represent all of the olefins because propene (PAR =1, OLE = 1) already was listed for background emissions. Dimethyl ether (PAR = 5, ALD2 = 1) was used to represent the higher aldehyde species (ALD2). The remaining portion of the paraffin bond group (after 1-butene and dimethyl ether were subtracted from it) was represented by an even split between iso-pentane (PAR=5) and n-pentane (PAR=5). The toluene bond group and isoprene bond group were represented by toluene and isoprene, respectively. The xylene bond group was broken up evenly and represented by m-xylene, o-xylene, and p-xylene in the MCM. The background emissions were assumed to be constant throughout the day and night.

	Background Emissions (tonnes/yr)	
Species Name	**ACBM (Jacobson 2007)**	**MCM (Carter 2008)**
Carbon Monoxide	285,000	285,000
Nitrogen Dioxide	170,100	170,100
Nitric Oxide	17,010	17,010
Methane	198,000	198,000
Ethane	17,200	17,200
Propane	4,890	4,890
Paraffin bond group (PAR)	115,000	
Iso-Pentane		9,016
N-pentane (pentane)		9,016
Ethene	10,100	10,100
Propene	1,680	1,680
1,3 Butadiene	718	718
Olefin bond group (OLE)	2,220	
1-Butene		2,220
Methanol	550	550
Ethanol	4,720	4,720
Formaldehyde	2,380	2,380
Acetaldehyde	631	631
Higher Aldehydes (ALD2)	4,080	
dimethyl ether		4,080
Formic Acid	139	139
Acetic acid	246	246
Acetone	2,920	2,920
Benzene	2,550	2,550
Toluene bond group	26,800	
Toluene		26,800
Xylene bond group	12,400	
m-Xylene		4,133
o-Xylene		4,133
p-Xylene		4,133
Isoprene bond group	134	
Isoperene		134
Unreactive	28,600	28,600
Sulfur Oxides as SO2	22,700	22,700
Ammonia	28,900	28,900

Table S14: Background Emission for SCAB for ACBM and MCM from Jacobson (2007a) and using Carter (2008)

Data was taken from the California Air Resources Board (CARB) to determine what the initialized background concentrations should be for the baseline case (CARB 2008). The sensitivity to this parameter was investigated by examining a range of initial conditions because it is difficult to predict what the concentrations of these species will be in 2020, when this simulation is taking place. Looking at the sensitivity of the results to background initial conditions also provides a clue to how the results would differ in different urban areas. The data at 6 am for a week in July and a week in August in 2008 was taken from the CARB database, shown in Table S15 (CARB 2008).

		South Coast Air Basin at 6 am (ppb)														
		Carbon monoxide			Nitrogen Dioxide			Nitric Oxide			Ozone			Sulfur Dioxide		
Day	Date	Max	Min	Avg	Max	Min	Avg	Max	Min	Avg	Max	Min	Avg	Max	Min	Avg
Th	7/10/2008	1000	200	430.4	32	4	21.6	58	1	21.0	58	1	12.9	3	1	2.00
F	7/11/2008	1200	200	486.4	38	0	22.5	64	0	20.0	41	2	10.9	4	1	2.00
S	7/12/2008	1100	100	404.3	32	3	16.4	49	2	14.1	42	3	10.6	4	0	2.29
Sun	7/13/2008	1000	100	362.5	28	3	13.9	46	0	10.7	52	4	14.3	3	0	1.86
M	7/14/2008	1000	200	480.0	39	7	21.0	97	2	23.9	31	1	10.3	4	1	2.43
T	7/15/2008	1000	200	508.0	45	8	25.4	99	3	29.5	25	1	9.7	5	1	2.57
	Average			445.3			20.1			19.9			11.4			2.19
Sun	8/10/2008	1000	100	412	31	1	17.1	48	1	13.6	42	5	12.4	6	0	1.71
M	8/11/2008	1000	100	464	36	5	20.4	70	0	26.0	33	1	10.2	5	0	2.14
Tu	8/12/2008	1100	100	432	43	2	22.9	107	0	21.5	38	2	10.4	5	0	1.86
W	8/13/2008	1000	100	476	35	8	23.3	71	2	23.8	32	1	9.8	6	0	1.71
Th	8/14/2008	800	0	384	36	7	22.0	50	1	15.5	33	2	10.0	7	0	2.14
F	8/15/2008	900	100	452	51	2	24.0	105	0	26.1	36	1	9.8	6	0	2.00
	Average			436.7			21.6			21.1			10.4			1.93

Table S15: Data from CARB on the Ambient Concentration of Select Species at 6 am for the SCAB (CARB 2008)

The average concentration, in ppbv, for those two weeks was used for the baseline for the species that are measured: carbon monoxide (CO) ~ 440 ppbv, ozone (O_3) ~ 10 ppbv, sulfur dioxide (SO_2) ~ 2 ppbv, nitric oxide (NO) ~ 20 ppbv, nitrogen dioxide (NO_2) ~ 20 ppbv (see Table S17). Unfortunately, the organic species were not measured for the SCAB. To estimate the amount of methane and non-methane organic gases in the SCAB at 6 am, we used the data from the San Francisco and San Jose areas in July and August at 6 am instead, as shown in Table S16: methane (CH_4) ~ 2000 ppb, non-methane organic gases (NMOG) ~ 80 ppb. The non-methane organic gases were then broken up according to the median value from Table 3.3 in Jacobson (~~2005~~), which lists the background concentrations of different species in the polluted urban troposphere. Thus, we initialized the following NMOGs at the start of our model runs: methane (CH_4) ~ 2000 ppbv, Ethane (C_2H_6) = 11.83 ppbv, Ethene (C_2H_4) = 7.19 ppbv, formaldehyde (HCHO) = 46.61 ppbv, toluene = 7.19 ppbv, m-xylene = 2.4 ppbv, o-xylene = 2.4 ppbv, p-xylene = 2.4 ppbv. The sensitivity of the system to these parameters was investigated as discussed in detail in the main paper. The summary of the initial conditions are shown in Table S17.

At 6 am		San Jose (ppb)					San Francisco (ppb)
Day	Date	NMHC	CH4	CO	NO	NO2	NMHC
W	8/1/2007	30	1940	300	5	14	120
Th	8/2/2007	80	2020	400	10	19	80
F	8/3/2007						100
S	8/4/2007	230	2240	500	26	17	80
Sun	8/5/2007	0	1860	100	1	4	50
M	8/6/2007	10	1840	200	2	8	80
Tu	8/7/2007	10	1870	200	2	9	80
W	8/8/2007	80	1960	400	8	20	70
Th	8/9/2007	60	2050	300	5	16	90
F	8/10/2008	110	2190	400	27	20	90
S	8/11/2008	140	2490	400	22	18	60
Sun	8/12/2008	100	2070	300	3	12	50
Average		77.3	2048.2	318.2	10.1	14.3	79.2

Table S16: Data from CARB on the Ambient Concentration of Select Species at 6 am for San Jose and San Francisco (CARB 2008)

	Initial concentrations (ppb)				
Species	**-20%**	**-10%**	**Baseline**	**+10%**	**+20%**
Carbon Monoxide			**440**		
Ozone			**10**		
Sulfur Dioxide			**2**		
Nitric Oxide	16	18	**20**	22	24
Nitrogen Dioxide	16	18	**20**	22	24
NMOG	64	72	**80**	88	96
Methane			**2000**		
Ethane	9.46	10.6	**11.83**	13.0	14.2
Ethene	5.75	6.47	**7.19**	7.91	8.63
Formaldehyde	37.3	41.9	**46.61**	51.3	55.9
Toluene	5.75	6.47	**7.19**	7.91	8.63
o-Xylene	1.92	2.16	**2.40**	2.64	2.88
m-Xylene	1.92	2.16	**2.40**	2.64	2.88
p-Xylene	1.92	2.16	**2.40**	2.64	2.88

Table S17: The Initial Concentrations for the Model – Baseline and Variations On the Baseline Used to Test the Sensitivity of the Model Results to Initial Conditions

4. Results

The model was run for a variety of ambient temperature profiles, as shown in Figure S15, for two days for all four emissions sets (gasoline and E85, both taken at 24 C and -7 C). Figure S18, Figure S19, and Figure S22show results from the two day model runs for a few select species for the warm temperature profiles (above freezing) and the 24 C data sets. Figure S20, Figure S21, and Figure S23 show the same for the cold temperature profiles (below freezing) and the -7 C data sets.

These time-series results indicate how the species concentration changed throughout the day and how the ambient temperature impacted the magnitudes of the species peaks. Note that the scale is different for different species, but the same for both E85 and gasoline for the same species and temperatures to allow for easy comparisons. The results show the typical peak of ozone and peroxy acetyl nitrate (PAN) in the afternoon, with an early morning peak in nitric oxide (NO), when these peaks are often observed in the urban environment. Ozone's peak mixing ratio generally increases with increasing temperature (Figure S22 and Figure S23). PAN increases with increasing temperature for cold temperatures, but starts decreasing around 13 C when the temperatures are warm enough that PAN's destruction dominates over its creation. The organic species, such as ethanol, formaldehyde (HCHO), acetaldehyde (CH_3CHO), toluene, and 1, 3-butadiene, are less sensitive to temperature, particularly to cold temperature.

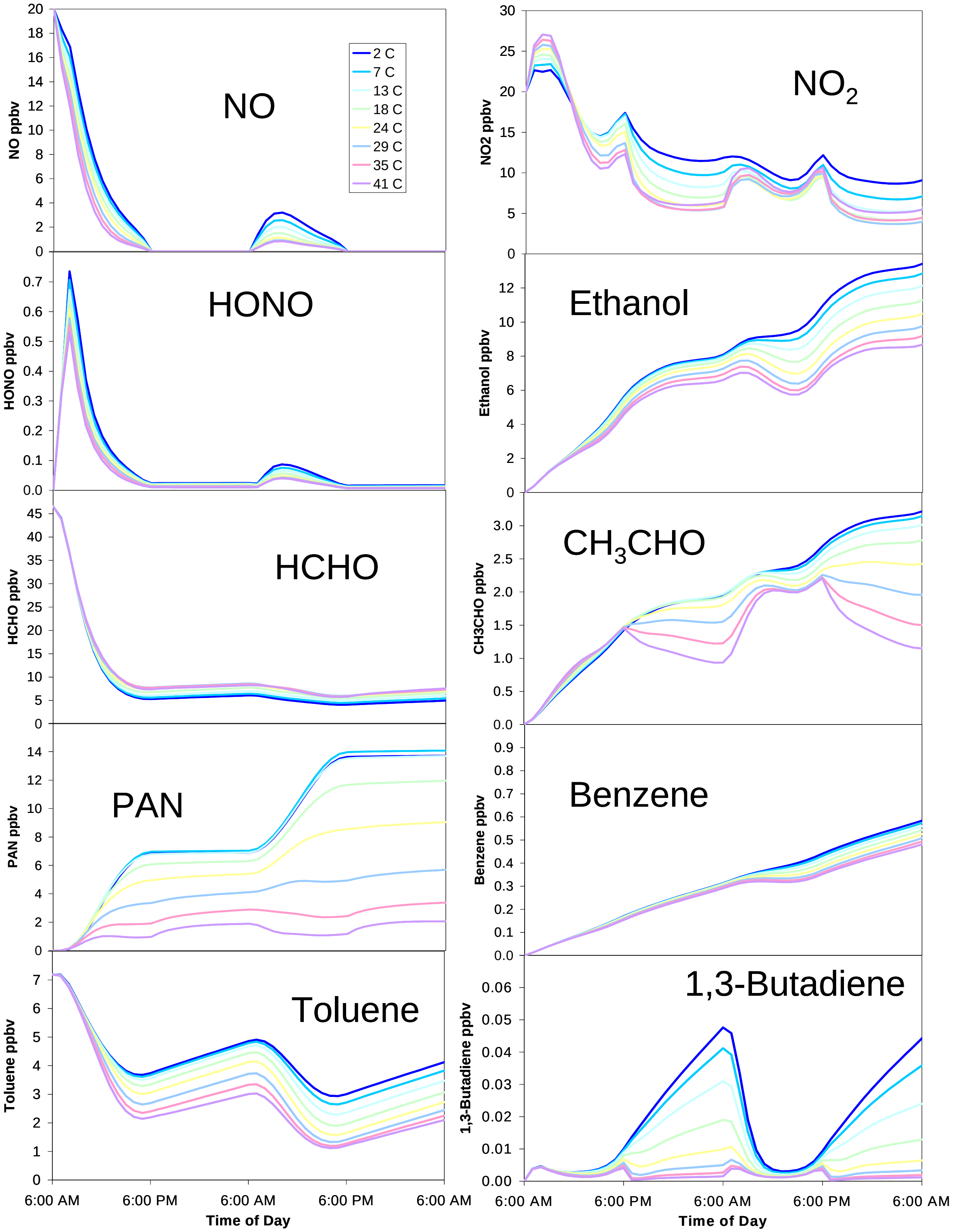

Figure S18: Two Day Model Results for E85 Emissions (24 C) for 8 Different Ambient Temperature Profiles

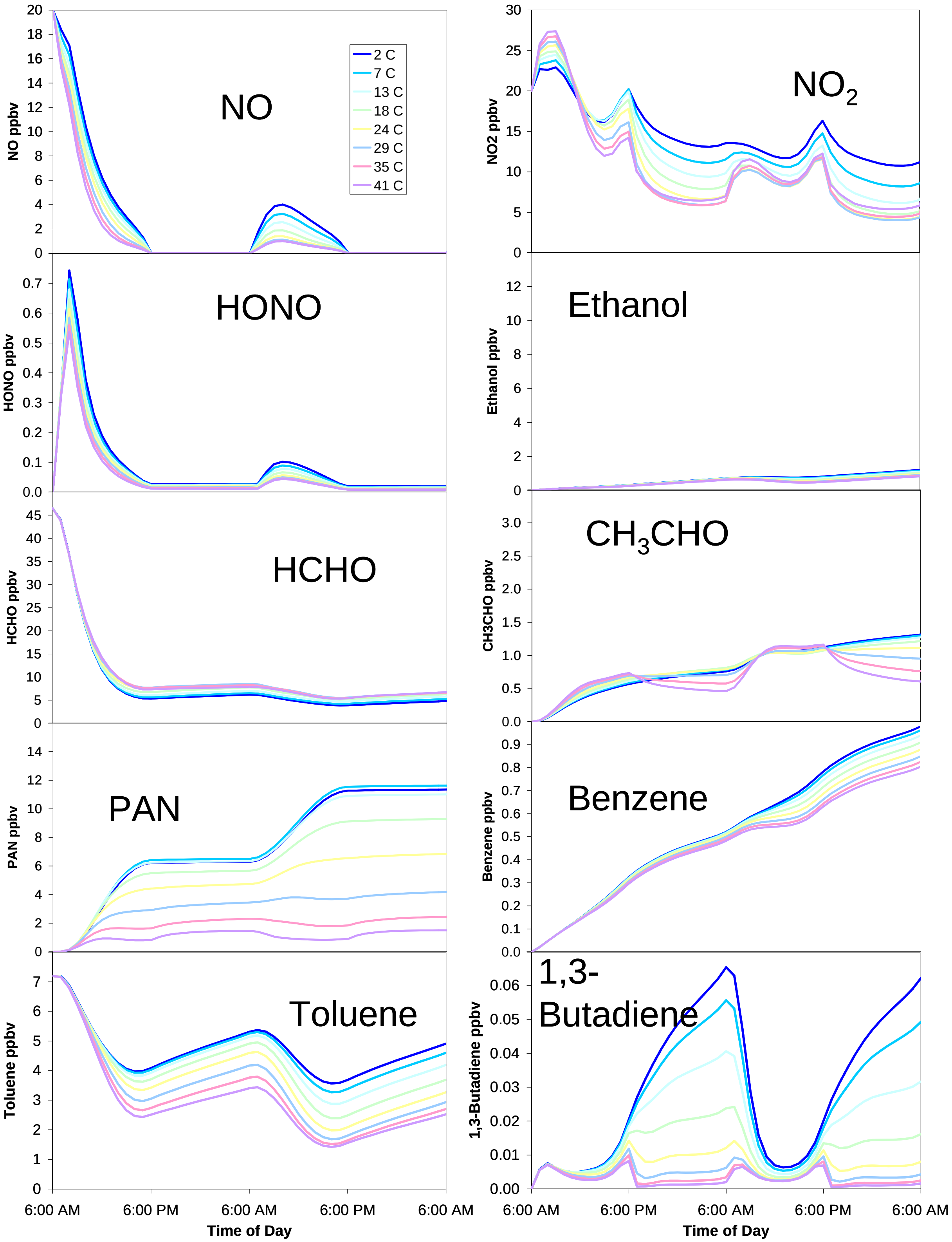

Figure S19: Two Day Model Results for Gasoline Emissions (24 C) for 8 Different Ambient Temperature Profiles

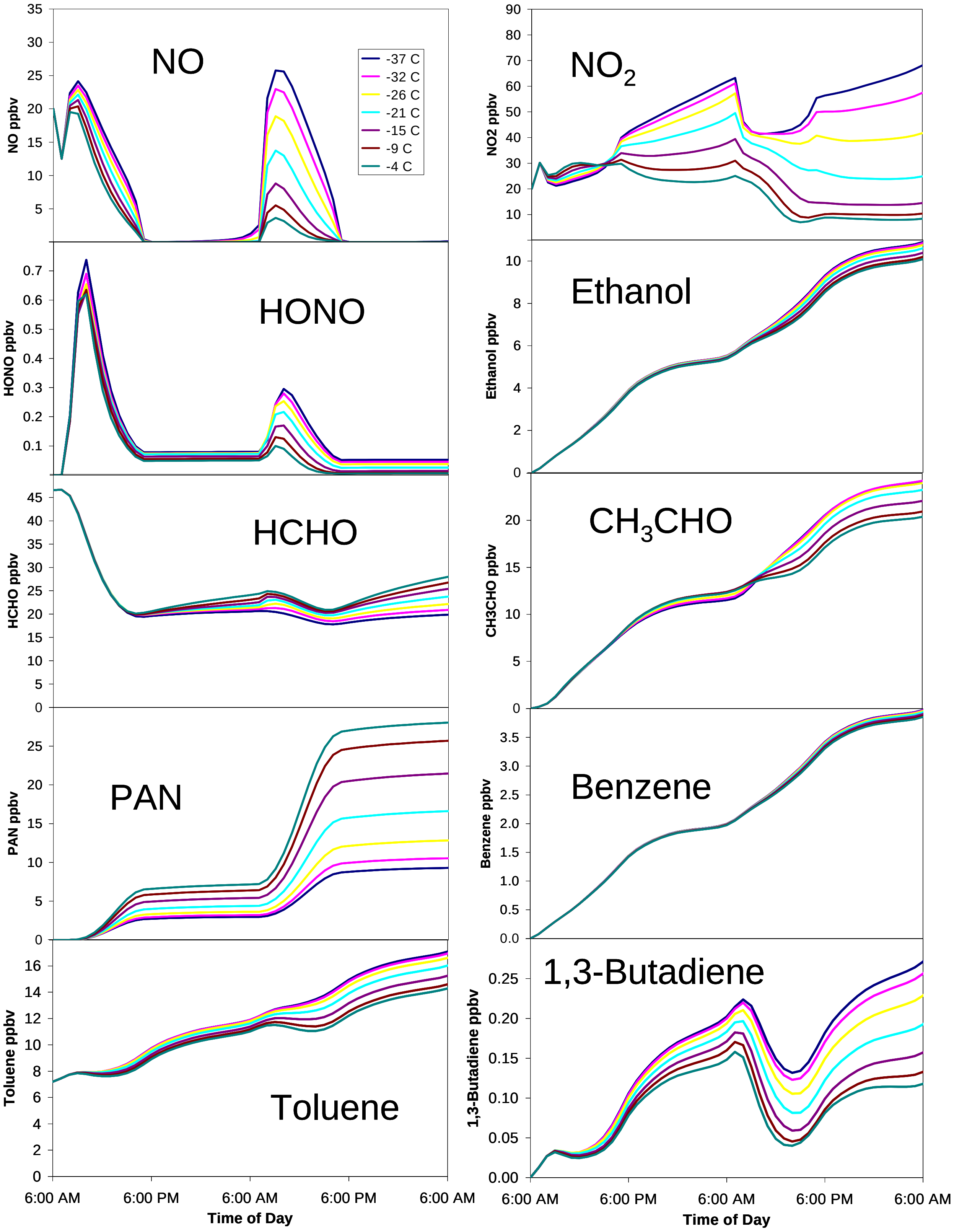

Figure S20: Two Day Model Results for E85 Emissions (-7 C) for 7 Different Ambient Temperature Profiles

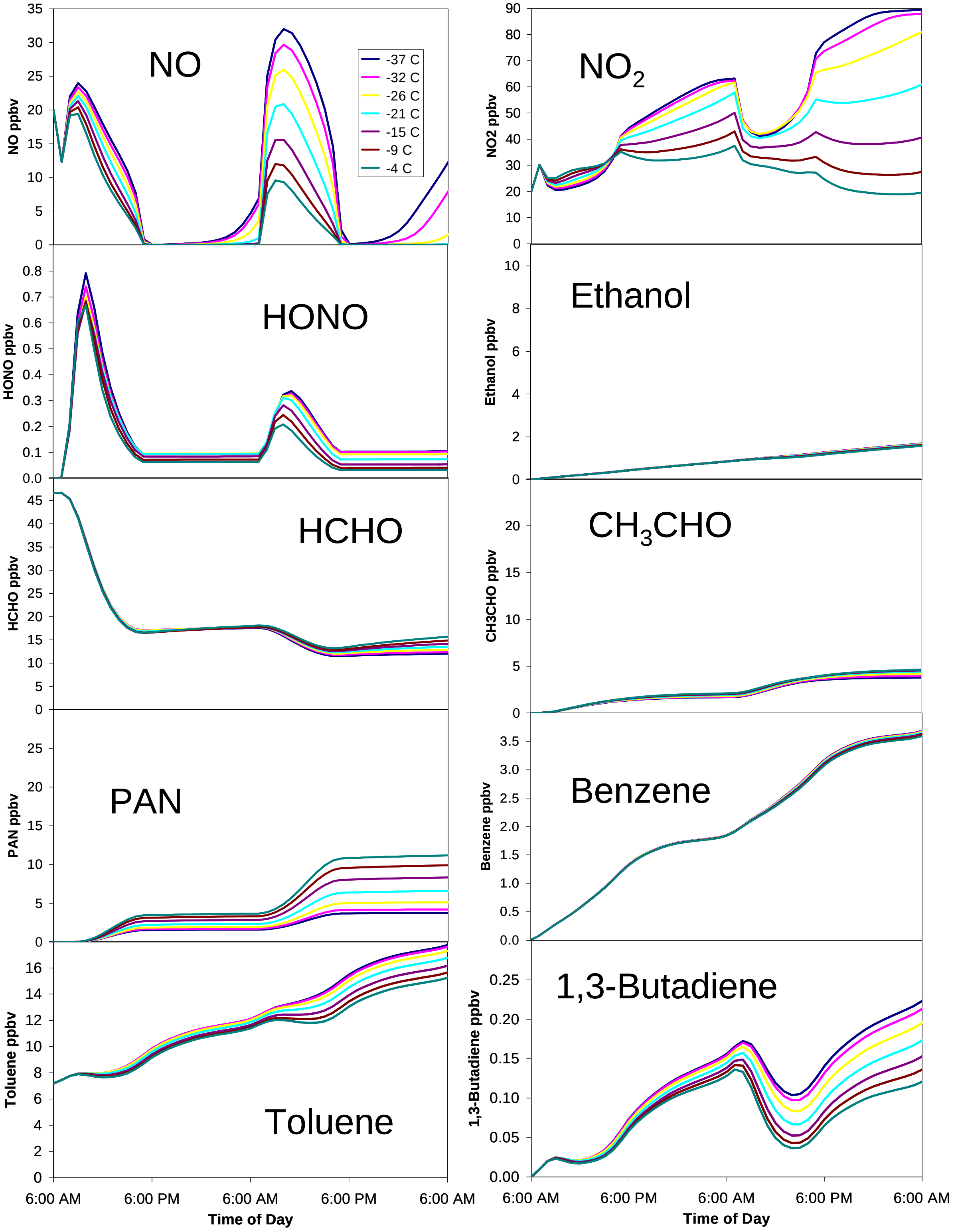

Figure S21: Two Day Model Results for Gasoline Emissions (-7 C) for 7 Different Ambient Temperature Profiles

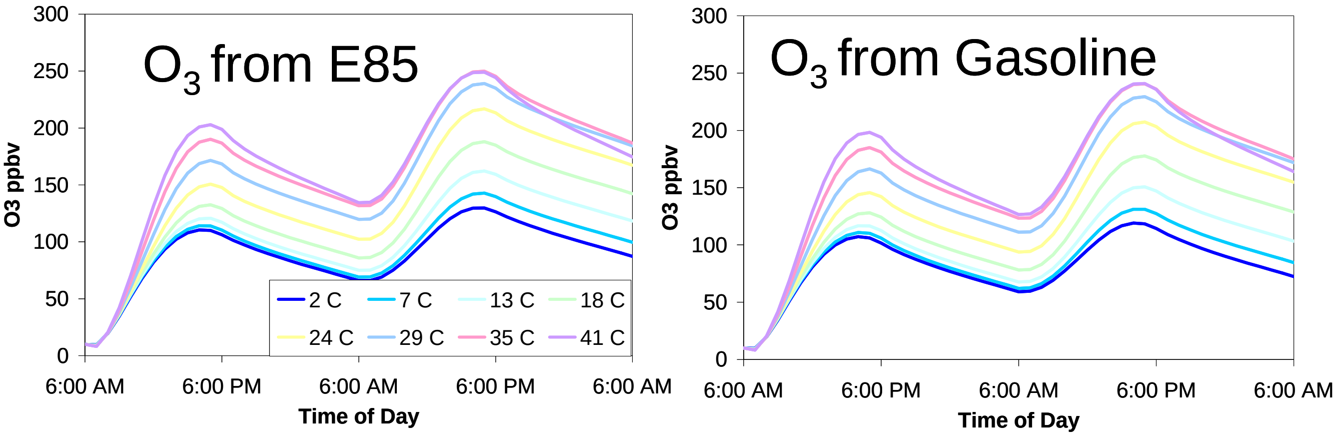

Figure S22: Two Day Model Results for Ozone from E85 and Gasoline 24 C Emissions Data for 8 Different Ambient Temperature Profiles

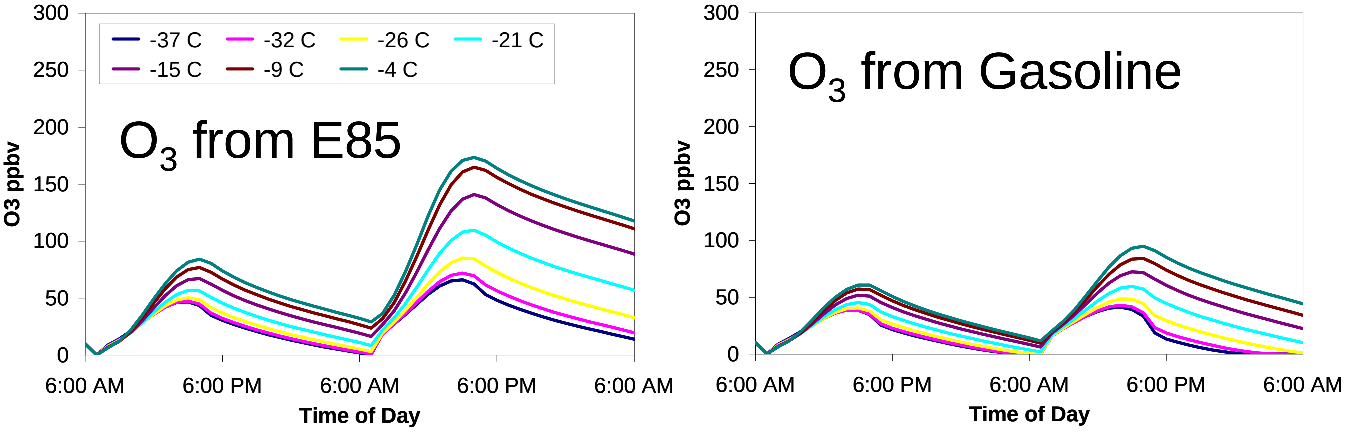

Figure S23: Two Day Model Results for Ozone from E85 and Gasoline -7 C Emissions Data for 7 Different Ambient Temperature Profiles

The ozone isopleth describes the change in ozone concentration as the NOx/VOC ratio changes, as shown in Figure S24. When the NOx/VOC ratio is high, the atmosphere is in the upper triangle of Figure S24 and a small change in VOCs can have a large impact on the ozone concentration. With a low NOx/VOC ratio, in the lower triangle of Figure S24, a large change in VOCs have little to no impact on ozone concentrations.

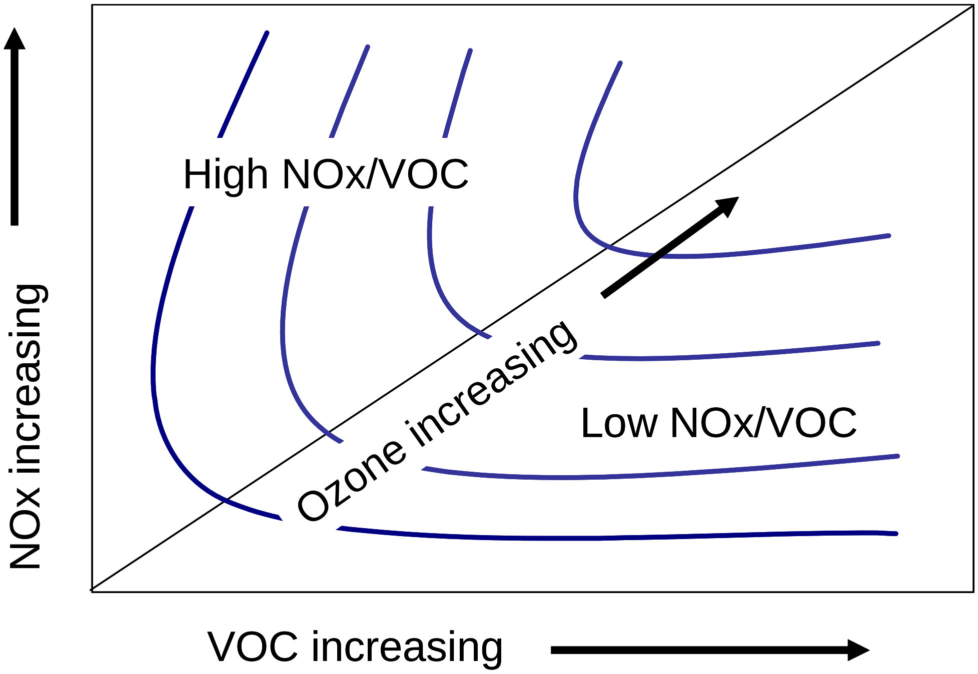

Figure S24: General Illustration of an Ozone Isopleth

5. Model Sensitivity

The sensitivity tests are described in detail in the main paper along with the results for the 24 C emissions. The differences between the average ozone for E85 and gasoline for each case are described and displayed in Figure 4. The actual average ozone results are shown here in Figure S25. The same sensitivities were also investigated for the -7 C emissions using the -4 C temperature profile, shown in Figure S26 and Figure S28, and are discussed more here.

For box height (mixing height), in the red square in Figure S26, the baseline was set at 500m. With the box height at 300m, ozone decreased for gasoline and increased for E85, increasing the difference from 39.4 ppbv to 65.9 ppbv. The average ozone increased for gasoline and decreased for E85 with the box height set to 1km, decreasing the difference to 13.9 ppbv. The box height seemed to have more impact on the average ozone concentration from gasoline than from E85 for the -7 C emissions.

The background water vapor concentration also had more impact on gasoline ozone than E85 ozone, but the impact of water vapor at the cold temperatures was not significant. A slight decrease of 4.2 ppbv in the difference from the baseline to the higher water vapor case was observed. The lower water vapor case caused a slight increase in the difference of 1.7 ppbv.

The initial background levels of NOx were modified, shown in the green box in Figure S26. Increasing or decreasing the NOx ratio had very little impact on the average ozone concentrations or the difference between E85 and gasoline.

Next, initial NOx concentration was changed by +20%, +10%, -10%, and -20%, giving initial background NOx concentrations of 48 ppbv, 44 ppbv, 36 ppbv, and 32 ppbv (ratio was 50/50). Increasing overall initial NOx by 20% and 10% decreased the average ozone and increased the difference by 5.1 ppbv and 2.8 ppbv, respectively (Figure S26). Average ozone increased when NOx was decreased by -10% and by -20% for both gasoline and E85, but it increased more dramatically for gasoline, decreasing the difference by 3.1 ppbv and 6.3 ppbv.

This suggests that the system is in the upper half of the ozone isopleth, shown in Figure S24, because a decrease in NOx increases ozone concentrations.

Four sensitivity cases were tested for the initial background concentrations of NMOGs: +20%, +10%, -10%, -20%. The results are shown in the purple box in Figure S26. Increasing initial NMOGs increases average ozone concentrations for both gasoline and E85. When initial background concentrations of NMOGs were decreased, average ozone also decreased. The impact is more dramatic on gasoline, which leads to a slight decrease in the difference when NMOGs are increased and an increase in the difference when NMOGs are decreased.

The sensitivities of the -7 C system to background emissions, background NOx emissions, and toluene are shown Figure S28. Decreasing the overall background emissions or the background NOx emissions also decreases the difference in average ozone concentration between E85 and gasoline. The average ozone concentration increases in these cases, again more dramatically for gasoline than for E85. The opposite trend is observed for increasing background emissions, with gasoline again impacted more strongly.

Toluene sensitivity was also tested. As shown during the model validation, the MCM v.3.1 tends to over predict ozone concentrations from toluene. This makes it important to determine how much toluene impacts the results. First, the initial background toluene was set to zero. This lowered the average ozone concentrations, especially for gasoline, increasing the difference between E85 and gasoline by 5.4 ppbv. Doubling the initial background toluene increased the average ozone concentrations and decreased the difference between E85 and gasoline by 6.5 ppbv. The toluene background emissions had very little impact on average ozone levels.

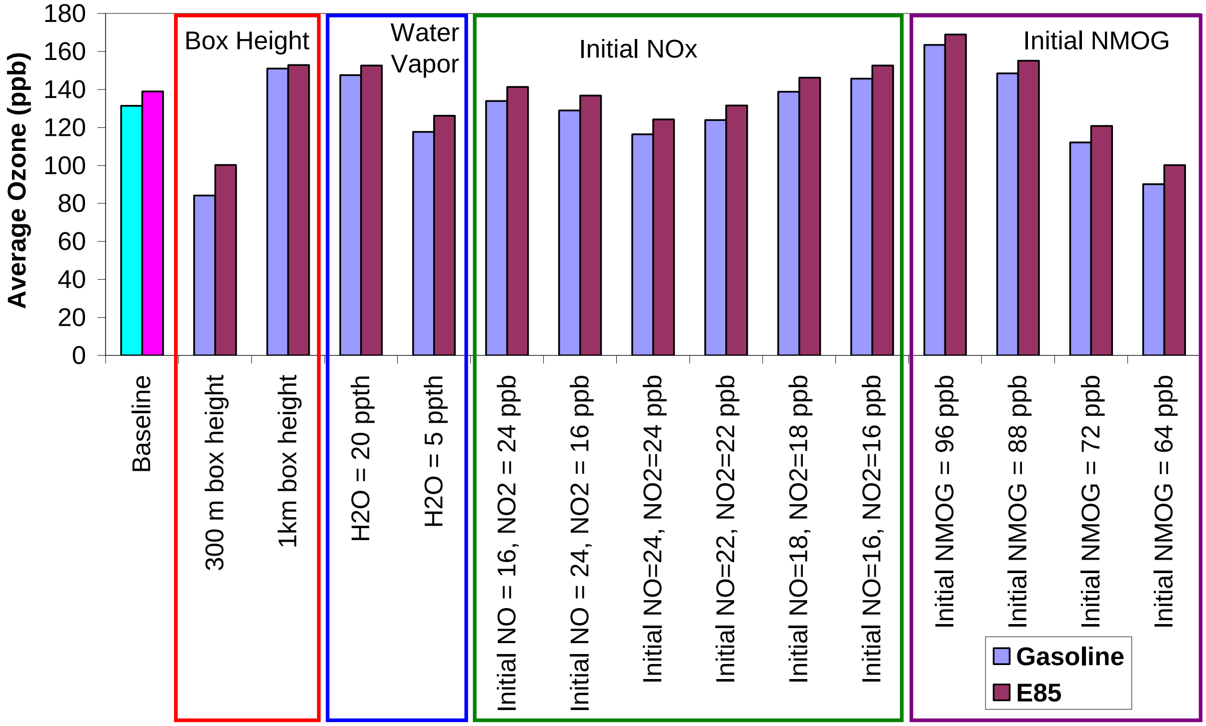

Figure S25: Two Day Average Ozone Concentration for E85 and Gasoline to Test the Model's Sensitivity to Box Height, Water Vapor, Initial NOx and Initial NMOG, Modeled at 24 C using the 24 C Emissions Set

Note: Baseline has a box height of 500 m, H_2O = 10 ppth, Initial NO = 20 ppbv, Initial NO_2 = 20 ppbv, Initial NMOG = 80 ppbv

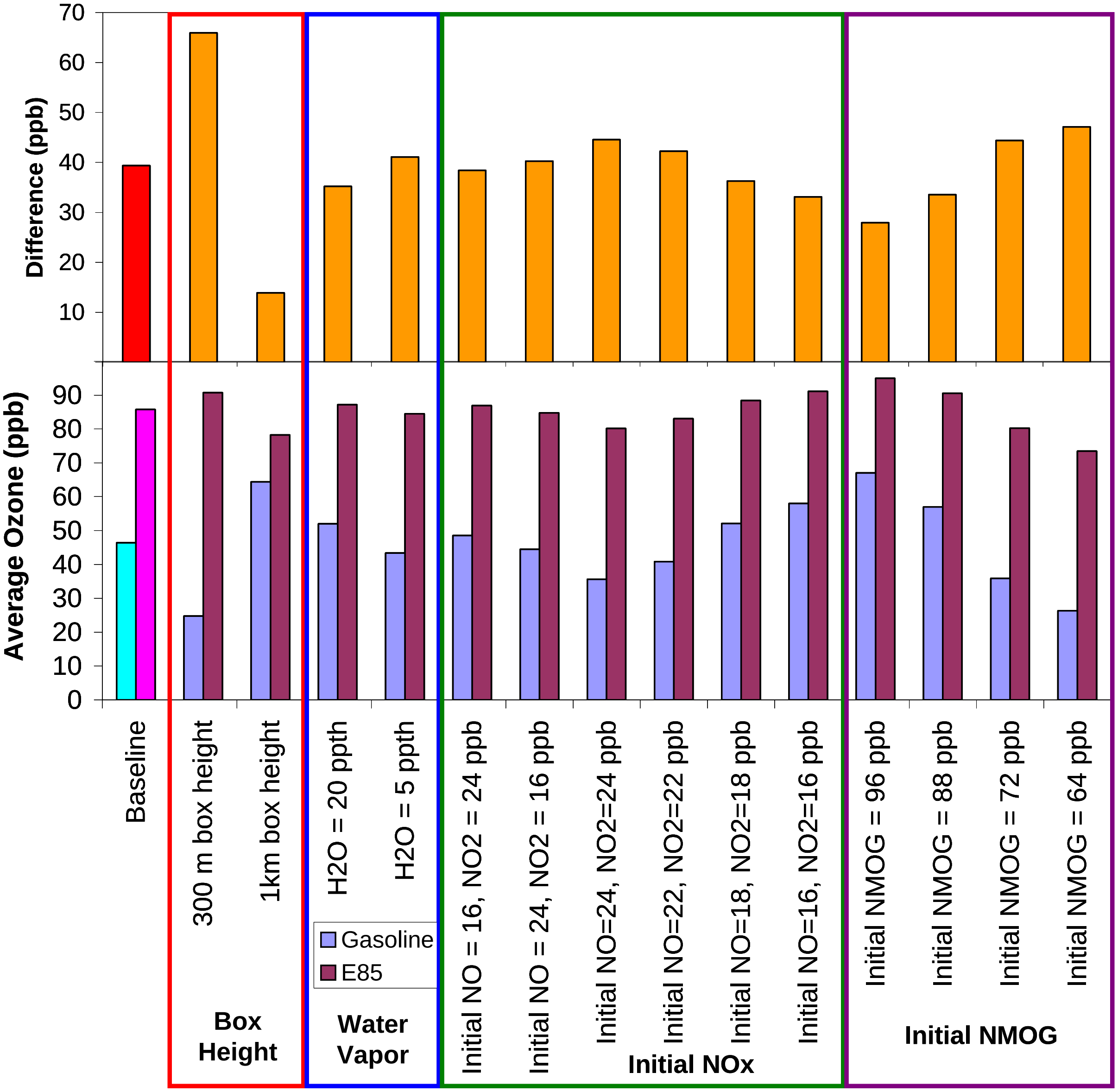

Figure S26: Difference in Two Day Average Ozone Concentration (E85 – Gasoline) (top figure) and Two Day Average Ozone Concentration for E85 and Gasoline (bottom figure) to Test the Model's Sensitivity to Box Height, Water Vapor, Initial NOx and Initial NMOG, Modeled at -4 C using the -7 C Emissions Set

Note: Baseline has a box height of 500 m, H_2O = 10 ppth, Initial NO = 20 ppbv, Initial NO_2 = 20 ppbv, Initial NMOG = 80 ppbv

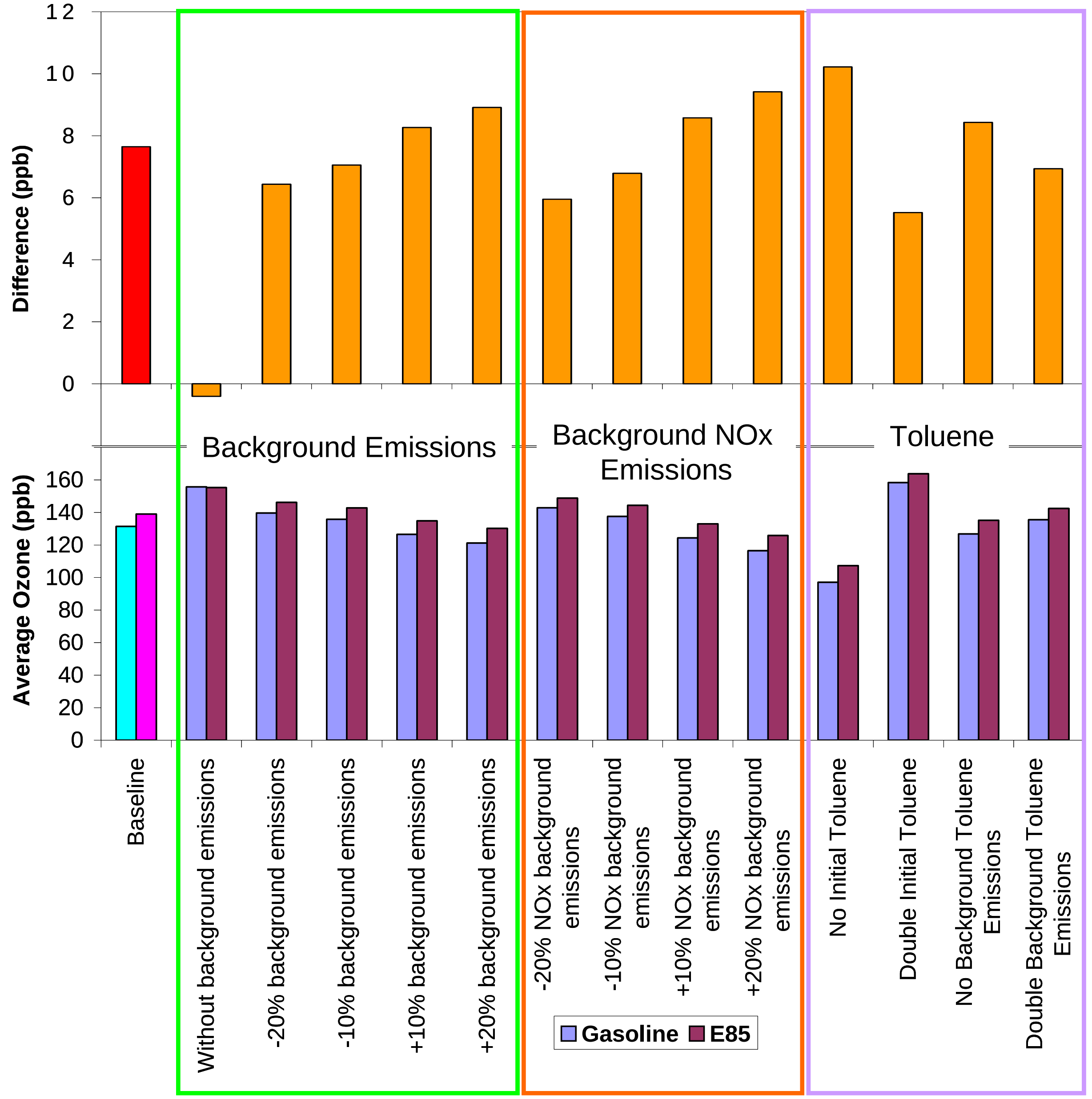

Figure S27: Difference in Two Day Average Ozone Concentration (E85 – Gasoline) (top figure) and Two Day Average Ozone Concentration for E85 and Gasoline (bottom figure) to Test the Model's Sensitivity to Total Background Emissions, Background NOx Emissions, and Toluene, Modeled at 24 C using the 24 C Emissions Set

Note: Baseline has a box height of 500 m, H_2O = 10 ppth, Initial NO = 20 ppbv, Initial NO_2 = 20 ppbv, Initial NMOG = 80 ppbv

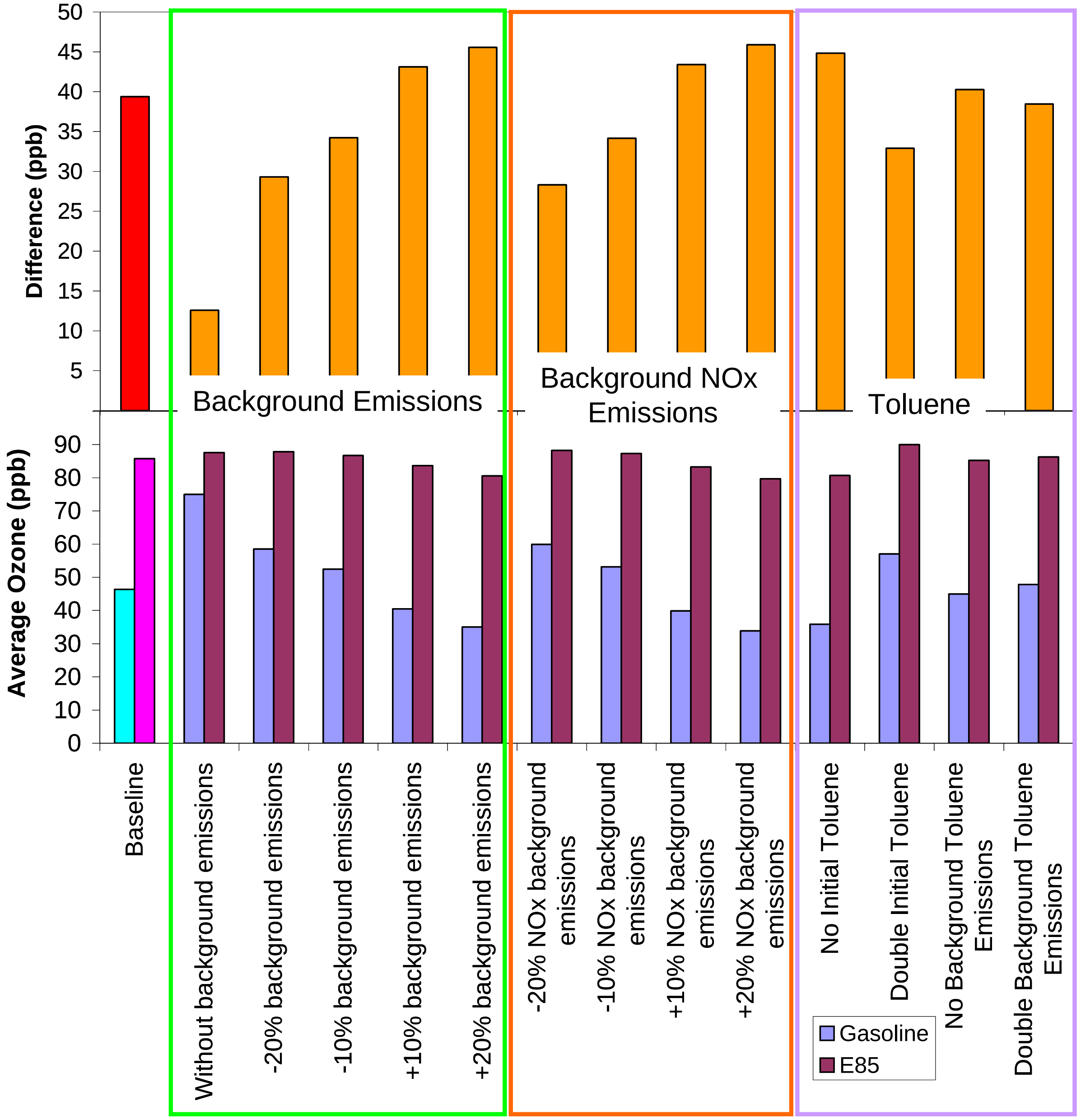

Figure S28: Difference in Two Day Average Ozone Concentration (E85 – Gasoline) (top figure) and Two Day Average Ozone Concentration for E85 and Gasoline (bottom figure) to Test the Model's Sensitivity to Total Background Emissions, Background NOx Emissions, and Toluene, Modeled at -4 C using the -7 C Emissions Set

Note: Baseline has a box height of 500 m, H_2O = 10 ppth, Initial NO = 20 ppbv, Initial NO_2 = 20 ppbv, Initial NMOG = 80 ppbv

Summary

Here we have provided detailed background information on the emissions and model used for this study along with additional information about the speed and accuracy of the model. The speed and accuracy conclusions discussed here are supported by our recent study (Jacobson and Ginnebaugh ~~2009~~) where the MCM v. 3.1 was found to provide more accurate ozone predictions than the ACBM and the SMVGEAR II solver was able to solve the MCM v.3.1 in a

3-D model with reasonable computer runtimes. In addition, we have shown that E85 may increase urban ozone concentrations over gasoline through a variety of scenarios. The increase is particularly marked at colder temperatures, which may have significant implications for winter time use of E85 and the potential impact to human health.

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