

Final Report

HARC Project H-8B

**Effect of Hotsoak and Diurnal Emissions
Spatial Allocation Methodology On Predicted Ozone Levels**

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Certification

The Contractor, ENVIRON International Corp., hereby declares that, to the best of its knowledge and belief, the information provided herein under Contract Number # H8B-2003-SPA is complete, accurate and complies with all of the requirements of the contract.

Date: 19 August 2003

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EXECUTIVE SUMMARY

Emission inventories are a major factor influencing the pollutant concentrations as predicted by photochemical models. Except for the Dallas/Fort-Worth (DFW) area, the emission inventories for Texas have historically been developed such that the on-road evaporative hydrocarbon emissions have been spatially allocated based upon link vehicle miles traveled (VMT) data. This tends to concentrate these emissions in urban areas where most of the travel network VMT occurs and within these, frequently to specific grid cells containing major freeways and arterials. This may lead to concentration spikes that are not reflective of actual conditions. On the other hand, inventories for the DFW non-attainment area State Implementation Plan, as developed by the North Central Texas Council of Governments, utilized a more detailed zone-based approach, in which evaporative hotsoak and diurnal emissions were spatially allocated to trip ends. The zone-based approach is more realistic because hotsoak and diurnal emissions occur when the vehicle is parked. EPA's latest on-road mobile emission factor model, MOBILE6, shows evaporative emissions increasing in significance as exhaust emissions are being reduced over time. Thus the ratio of evaporative to exhaust emissions using MOBILE6 is higher than using MOBILE5 in future year modeling. The objective of this project was to determine the impacts upon modeling results associated with the two spatial allocation approaches for hotsoak and diurnal emissions, including the effects of recent updates in the emissions modeling tool, MOBILE.

To perform assessments of the impact of allocation methodology and model updates, the existing 1995 DFW SIP episodic modeling inventory, adjusted to 2007 levels, was selected. The 2007 inventory was then modified to yield MOBILE5- and MOBILE6-based inventories with the hotsoak and diurnal portions spatially allocated through both link- and zone-based approaches. Each of these inventories was then input into the CAMx photochemical model for the 1995 DFW SIP ozone episode.

The modeling results were interpreted to assess whether the refinements in emissions methodology are a significant improvement, what magnitude impacts are to be expected and under what conditions the impacts will be most significant. A summary of the results is presented here:

- The zone-based allocation methodology resulted in higher emissions concentrations. The explanation for this that the zone-based emissions were originally concentrated in a handful of travel analysis zones (TAZs) which are not significantly larger than a 4km grid cell. Thus, when these emissions were summed throughout a county and redistributed over the entire travel network spanning a large number of grid cells the net result is dispersion of the emissions.
- Differences in modeled maximum daily ozone concentrations between the two allocation methodologies were small, on the order of tenths of a ppb. The differences for the MOBILE6-based scenarios were larger than the MOBILE5-based scenarios consistent with MOBILE6 having a higher ratio of evaporative to exhaust VOC emissions than MOBILE5.
- In most instances, the choice of allocation methodology did not change the location of the maximum ozone. The only exception was the first episode day (during which the

largest differences in daily maxima occurred). However, results from the first day of an ozone model run normally are not considered reliable because of the influence of the initial condition assumptions.

- The peak ozone for the episode did not change significantly from 124 ppb under any scenario, i.e., link or zone-based evaporative emissions with MOBILE5 or MOBILE6.

From these findings, it is concluded that the modeled impacts depend upon the relative contribution of affected emissions, the size and location of zones used to allocate hotsoak and diurnal emissions, and the sensitivity of local ozone levels to VOC versus NO_x. In the absence of strong synergies between these aspects, significant impacts on modeled ozone levels from the choice of allocation methodology are unlikely.

1. INTRODUCTION

The purpose of this work was to determine the sensitivity of modeled ambient ozone concentrations to the spatial allocation of ozone precursor emissions from on-road mobile sources. In particular, the effect of the choice of methodology used to spatially distribute hot soak and diurnal emissions from on-road vehicles was examined using an existing MOBILE5-based 2007 emission inventory developed by the North Central Texas Council of Governments (NCTCOG) for the Dallas/Fort-Worth (DFW) area. This base inventory, in which the diurnal and hot soak emissions were allocated using traffic analysis zones (TAZ), was modified such that these same emissions were distributed to travel network links. These inventories were also each converted to a MOBILE6 basis to study the significance of the spatial allocation effect when this version of MOBILE, which has a higher evaporative-to-exhaust ratio, is used to develop the emissions.

This technical report describes how the 2007 DFW (base) emission inventory was modified for each of four modeling scenarios:

1. MOBILE5-based with hot soak and diurnal emissions allocated based on TAZs (this scenario, though already represented in the existing base inventory, was reprocessed to ensure compatibility with inventory,
2. MOBILE5-based with hot soak and diurnal emissions allocated based on vehicle miles traveled (VMT) on specific travel network links,
3. MOBILE6-based with hot soak and diurnal emissions allocated based on TAZs, and
4. MOBILE6-based with hot soak and diurnal emissions allocated based on VMT on specific travel network links. The assumptions used to produce the final modeling inventories are documented and the photochemical modeling results are also presented and discussed.

2. APPROACH

Dallas/Fort-Worth (DFW) was selected for the analysis, rather than Houston, because mobile sources contribute a greater proportion of ozone precursor emissions in DFW than Houston. We began with existing MOBILE5-based SIP modeling inventories for a June 18-22, 1995 ozone episode that were projected to 2007 levels by NCTCOG. The Texas Commission on Environmental Quality (TCEQ) also modeled a 1996 episode for the DFW SIP, but the mobile source emissions are more difficult to quantify for this episode because it included a July 4th holiday. Thus, we considered the June 1995 episode to be a better candidate for evaluating the impacts of the proposed refinement of the mobile emissions modeling methodology.

The TCEQ has begun developing a new ozone model for DFW for a 1999 episode. The new DFW episode will have MOBILE6-based emissions, but these emissions and ozone modeling databases were not ready in time for this project.

Three independent modifications/improvements were implemented to produce four alternative model-ready inventories. These are as follows:

1. Spatially allocate MOBILE5-based evaporative emissions (hotsoak and diurnal) to travel analysis zones (TAZs). This is the base inventory approach used by NCTCOG (1998).
2. Spatially allocate MOBILE5-based evaporative emissions (hot soak and diurnal) using link-based VMT
3. Estimate exhaust and evaporative emissions using MOBILE6/MOBILE5 ratios (in essence transforming current inventories to a MOBILE6 basis) but keeping the zone-based allocation scheme
4. Estimate exhaust and evaporative emissions using MOBILE6/MOBILE5 ratios, then spatially allocate the MOBILE6-based evaporative hot soak and diurnal emissions to links proportional to their associated VMT

To ensure consistency so that the modeling results are comparable, the alternative inventories were developed following NCTCOG methodology whenever possible. Where insufficient information exists to permit this, assumptions were made and these are mentioned below. For more detailed information on the development of the original NCTCOG on-road base inventory, see NCTCOG (1998).

REDISTRIBUTING HOT SOAK AND DIURNAL EMISSIONS WITHIN THE BASE INVENTORY

One of the major modifications employed in this work to produce alternative emission inventories is the redistribution of the hotsoak and diurnal emissions from TAZs to travel network links, i.e. roadway segments. The following discussion details the technique that was applied to both the base inventory and MOBILE6 zone-based inventory (the details of whose derivation from the base inventory are given in the next section) to produce the MOBILE5 and MOBILE6 link-based emissions inventories, respectively. Only gasoline vehicle types were assumed to have hotsoak and diurnal emissions. These vehicle classes include light-duty gas vehicles (LDGV), light-duty gas trucks less than 6000 lbs GVWR (LDGT1), light-duty gas

trucks between 6000 and 8500 lbs GVWR (LDGT2, heavy-duty gas vehicles (HDGV) and motorcycles (MC).

Diurnal and hotsoak emissions were separately summed across all TAZs within a county for each episode day. These emissions sums retained the distribution among vehicle classes as well as time-of-day (TOD) variation. Then the VMT was summed across all links within each county for each TOD. (Link-level VMT information was included along with the link-level emissions data provided by the NCTCOG). These VMT totals were then disaggregated to each of the five gasoline vehicle types based upon VMT mix fractions from the DFW 1995 inventory documentation (NCTCOG, 1998, see Table 2-1). These fleet mixes were available only for arterials and freeways. Therefore, the freeway VMT mix was also applied to ramps and HOV lanes while the arterial fleet mix was used to disaggregate VMT on collectors, locals, and frontage roads (in addition to arterials). Once the vehicle class-specific VMT was estimated for each link in each TOD period, the fraction of the total county VMT associated with each link was computed. This was done by vehicle class. Hotsoak and diurnal emissions associated within each county, vehicle and TOD were then distributed to each link based upon the fractions calculated above.

Table 2-1. VMT mixes used to assign link VMT to vehicle classes.

Vehicle Class	Urban Core Counties		Rural Core Counties	
	Freeway VMT mix	Arterial VMT mix	Freeway VMT mix	Arterial VMT mix
LDGV	0.619	0.669	0.610	0.618
LDGT1	0.181	0.177	0.184	0.186
LDGT2	0.111	0.108	0.109	0.110
HDGV	0.026	0.021	0.025	0.023
LDDV	0.003	0.004	0.004	0.004
LDDT	0.002	0.002	0.002	0.002
HDDV	0.054	0.014	0.063	0.052
MC	0.004	0.005	0.003	0.005

SCALING THE BASE INVENTORY TO MOBILE6.2 BASIS

The following discussion outlines the methodology for developing the 2007 on-road mobile source scaling factors between MOBILE6.2 and MOBILE5a_h, the version used by NCTCOG to develop the base inventory. The overall process to develop these scaling factors was consistent for link-based, local and diurnal/hotsoak emissions. The procedure includes modifying the NCTCOG base inventory input files to obtain comparable MOBILE6 files, which were run through MOBILE6.2. The MOBILE6.2 emission factors were ratioed to corresponding MOBILE5 emission factors to determine the scaling factors.

The core counties and the perimeter counties were modeled separately as more detailed data were available for the former. For the core counties, NCTCOG developed detailed 2007 emissions only for the first episode day (Monday, June 19). Emissions for the other episode days were estimated using a 'pivot methodology' that essentially scales the Monday emissions to the other days based upon the corresponding ratio of daily emissions from the 1995 inventory. Thus, the MOBILE6/MOBILE5 scaling factors for core counties were determined

for a single day (Monday) for each of 15 time periods or time-of-day (TOD). The perimeter counties were modeled as a single entity (i.e. using the same set of inputs) for each of the five episode days (Monday–Friday).

Core Counties

The DFW core counties for the 1995 inventory were Dallas, Tarrant, Collin, Denton and Rockwall. The base inventory's MOBILE5 input files were translated to MOBILE6 format using Route56 (ERG, 2001), a computer software developed by Energy Research Group to prepare MOBILE6 input files based upon existing MOBILE5 inputs, and then further modified to include scenarios covering a range of speeds (from 3 mph to 65 mph in increments of 1 mph) and roadway types. Most of the remaining original input parameters were retained. Separate MOBILE6 input files were generated for three roadway types: arterial, freeway and ramp and for the 15 time periods. Table 2-2 shows the modeling time period groupings. The rural (Collin, Denton, and Rockwall) and the urban counties (Dallas and Tarrant) were modeled separately.

Table 2-2. Modeling time period groupings.

TOD Number	Modeling Time Period
1	8 p.m. – 6 a.m.
2	6 a.m. – 7 a.m.
3	7 a.m. – 8 a.m.
4	8 a.m. – 9 a.m.
5	9 a.m. – 10 a.m.
6	10 a.m. – 11 a.m.
7	11 a.m. – 12 p.m.
8	12 p.m. – 1 p.m.
9	1 p.m. – 2 p.m.
10	2 p.m. – 3 p.m.
11	3 p.m. – 4 p.m.
12	4 p.m. – 5 p.m.
13	5 p.m. – 6 p.m.
14	6 p.m. – 7 p.m.
15	7 p.m. – 8 p.m.

For link-based emissions (which include exhaust, running loss, resting loss, and crankcase), scaling factors were derived for each road type, speed, vehicle class and pollutant. Note that MOBILE5 does not distinguish between roadway types; therefore, these scaling factors were determined by using a common set of MOBILE5 emission factors as the denominator. The scaling factors corresponding to arterials were used for principal/minor arterials, collectors, and frontage roads. The non-ramp (freeway) scaling factors were used for HOV lanes as well.

The scaling factors corresponding to local roads, while determined separately, were processed similarly to the link-based case except that the local road type input files were modeled using a single speed, 20 mph. (This speed was assumed by NCTCOG in developing the base emissions.) All the other base inputs were kept unchanged for the MOBILE6 modeling. The

base inventory's MOBILE5 input files were run through MOBILE5a_h. The exhaust CO, NOx and total VOC emission factors were obtained by vehicle class, TOD and county. The rural counties (Collins, Denton and Rockwall) were modeled together, while the urban counties (Dallas and Tarrant) were modeled as the other set. MOBILE6.2 input files were obtained from the base MOBILE5 files using the Route56 translator. The respective MOBILE6 outputs were divided by the MOBILE5 emission factors to obtain the scaling factors for emissions associated with local roads for the three pollutants (CO, NOx and VOC) and by time period (TOD1 to TOD15).

For hot soak and diurnal, MOBILE6 files for the two county groups were obtained by translating the relevant MOBILE5 input files using Route56. Since these emissions are independent of speed, they were modeled using a single scenario retaining the base inventory inputs. To estimate the diurnal/hot soak scaling factors, daily emission factors were extracted from the MOBILE6 and MOBILE5 runs for the urban and rural counties, and the ratios of the sum of diurnal and hot soak emission factors were used to scale both types of emissions. This is because in MOBILE5a_h, unlike other evaporative losses and exhaust emission factors which are expressed in grams/mile, diurnal and hotsoak emissions factors are reported in grams per day and per trip, respectively. The hotsoak + diurnal emission factor in grams/mile is thus obtained by subtracting the crankcase emission factor from the 'Evaporative HC' emission factor. Scaling factors for both diurnal and hot soak emissions were obtained for each of five gasoline vehicle classes (LDGV, LDGT1, LDGT2, HDGV, and MC).

Perimeter Counties

The 32-county perimeter region (NCTCOG, 1998) was modeled as a single set of inputs for each of the five episode days. Monday and Tuesday were modeled using the same temperature inputs while Wednesday, Thursday and Friday were modeled as a single climatic group.

To obtain the exhaust scaling factors for the perimeter counties, the MOBILE5 input files from the base inventory were first run for the two sets of episode days. The exhaust CO, NOx, VOC and the resting, running and crankcase emission factors were obtained from the MOBILE5 outputs. For MOBILE6.2, three sets of runs were developed for each of the three roadway types: freeway, arterial and local. This was done by translating the base MOBILE5 input files to MOBILE6 files using Route56 and modifying the runs for all three roadway types. Each run included scenarios for speeds ranging from 3 mph to 65 mph with increments of 1 mph. The scaling factors were calculated as the ratios between the corresponding MOBILE6 and MOBILE5 emission factors. Scaling factors developed from these ratios were by roadway type, vehicle class, pollutant, and episode day.

The evaporative scaling factors were obtained by summing the diurnal and hot soak emission factors from the MOBILE5 and MOBILE6 models. Since the MOBILE5 model reports hot soak and diurnal emission factors in units of grams and not grams/mile, the corresponding emission factors in grams/mile were obtained by subtracting the crankcase values from that of the total evaporative HC emission factors. MOBILE6 input files were generated from the base MOBILE5 files, and the sum of the hot soak and diurnal emissions (in grams/mile in MOBILE6) were divided by those from MOBILE5 to obtain the diurnal/hot soak scaling factors for the five gasoline vehicle classes. Since these emissions are independent of the

speed, each of the episodic input files was run for a single scenario without any speed command.

EPS2x PROCESSING OF EMISSIONS

The extended emissions processing system version 2 (EPS2x) was used to prepare model-ready emission inventories for each of the four scenarios listed above. Some adjustments were made to the emissions before input to EPS2x to account for local controls and other effects that cannot be modeled in MOBILE5 or 6. These across-the-board adjustments, which correspond to ‘Strategy 30’ (TNRCC, 2000), are based upon TCEQ’s methodology and are summarized in the table below. They include the effects of Tier2 emissions standards and fuel (applicable to MOBILE5-based inventories only), new CA LEV, CA diesel, transportation control measures (TCMs), Vehicle Recycling Program and others. (Refer to TCEQ (2003) for further information.)

Table 2-3. Adjustments to emissions prior to EPS2x processing.

Inventory	County	NOx adjust. factor	VOC adjust. factor
MOBILE5-based	Dallas & Tarrant	0.622	0.778
	Collin, Denton, Rockwall	0.542	0.532
	Ellis, Henderson, Hunt, Kaufman	0.478	0.393
	All others	0.708	0.860
MOBILE6-based	Dallas & Tarrant	0.786	0.810
	Collin, Denton, Rockwall	0.786	0.612
	Ellis, Henderson, Hunt, Kaufman	0.648	0.426
	All others	0.863	0.951

TCEQ provided most of the EPS2x setup used to process the base inventory and these specifications were followed whenever possible. Some noteworthy details of the EPS2x processing (especially where our processing deviated from that of TCEQ) are discussed below in sections specific to each EPS2x module.

LBASE Inputs

The LBASE module of EPS2x processes link-based emission and assigns them to grid cells. For link-based emissions, an input file for the LBASE module of EPS2x was generated for each day during the modeling period. The 2007 episodic emission inventories for the Dallas/Fort-Worth modeling domain have been prepared, as described above, for 15 time periods where TOD1 covers 8:00 PM to 6:00 AM while TOD2 to TOD15 correspond to each hourly period between 6:00 AM and 8:00 PM. Since the time interval for LBASE input records is typically set as one hour, emissions for the time period of TOD1 were disaggregated into 10 hourly amounts in proportion to the fraction of daily traffic associated with each hour in the time period (see Table 2-4). VOC emissions in the 2007 episodic emission inventories

were divided into exhaust, running loss, resting loss, and crankcase for each vehicle class. The crankcase emissions were added into the exhaust in the LBASE inputs.

PREAM Inputs

The PREAM module of EPS2x reads emission information that represents a geographic area, such as a county or TAZ. Input files for the PREAM module of EPS2x were made for both the zone-based core county emission files and county-level perimeter county emission files. For zone-based files, the zone number was used in place of a FIPS state/county codes. For the purpose of chemical speciation, VOC emissions for local roads, which were available only as totals, were divided into exhaust, running loss, resting loss, and crankcase portions using distribution profiles based on the link-based emissions (Table 2-5). As with the LBASE inputs, the crankcase emissions were added into the exhaust. For the perimeter counties, hot soak and diurnal emissions were given as total daily emissions. They were distributed into hourly emissions based on the daily traffic fractions (Table 2-4).

Table 2-4. Daily VMT distribution.

1995 and 1996 Episodic Emission Inventories	
Dallas-Fort Worth Modeling Domain: Core Counties	
	% of Daily Traffic
Hour of the Day	Weekday
12am – 1am	1.1 %
1am – 2am	0.7 %
2am – 3am	0.6 %
3am – 4am	0.5 %
4am – 5am	0.7 %
5am – 6am	2.0 %
6am – 7am	5.2 %
7am – 8am	7.4 %
8am – 9am	6.1 %
9am – 10am	4.9 %
10am – 11am	4.7 %
11am – 12pm	5.0 %
12pm – 1pm	5.3 %
1pm – 2pm	5.4 %
2pm – 3pm	5.8 %
3pm – 4pm	6.5 %
4pm – 5pm	7.5 %
5pm – 6pm	8.0 %
6pm – 7pm	6.5 %
7pm – 8pm	4.7 %
8pm – 9pm	3.6 %
9pm – 10pm	3.2 %
10pm – 11pm	2.7 %
11pm – 12am	1.9 %
Total	100 %

Table 2-5. Local roads VOC emission distributions by mode.

County Name	Emission Mode	Fraction
Collin	Exhaust	0.850
	Running loss	0.109
	Resting loss	0.034
	Crankcase	0.007
Denton	Exhaust	0.853
	Running loss	0.109
	Resting loss	0.031
	Crankcase	0.007
Dallas	Exhaust	0.834
	Running loss	0.122
	Resting loss	0.044
	Crankcase	0.000
Tarrant	Exhaust	0.834
	Running loss	0.122
	Resting loss	0.044
	Crankcase	0.000
Rockwall	Exhaust	0.850
	Running loss	0.100
	Resting loss	0.050
	Crankcase	0.000

CHMSPL

CHMSPL was used to chemically speciate both NO_x and VOC emissions. In all cases, we used more detailed area source codes (ASC) than were used by TCEQ in its preparation of the model-ready inventory from the base inventory. However, we used the TCEQ's speciation profiles for each fuel/vehicle type and emission mode. The ASC-speciation profile cross references are shown in the next table.

Table 2-6. Assignment of speciation profiles.

From TCEQ			ENVIRON		
ASC	Profile Code		ASC	Profile Code	
	Special Counties*	Other Counties		Special Counties*	Other Counties
MV01000EXH	D101	M115	MV01000EXH	D101	M115
			MV02000EXH	D101	M115
			MV03000EXH	D101	M115
			MV04000EXH	D101	M115
			MV08000EXH	D101	M115
MV05000EXH	D201	D201	MV05000EXH	D201	D201
			MV06000EXH	D201	D201
			MV07000EXH	D201	D201
			MV01000RST	D301	M141
MV01000RST	D301	M141	MV01000RST	D301	M141
			MV02000RST	D301	M141
			MV03000RST	D301	M141
			MV04000RST	D301	M141
			MV08000RST	D301	M141
MV01000EVP	D302	M151	MV01000RNL	D302	M151
			MV02000RNL	D302	M151
			MV03000RNL	D302	M151

From TCEQ			ENVIRON		
ASC	Profile Code		ASC	Profile Code	
	Special Counties*	Other Counties		Special Counties*	Other Counties
			MV04000RNL	D302	M151
			MV08000RNL	D302	M151
			MV01000HOT	D302	M151
			MV02000HOT	D302	M151
			MV03000HOT	D302	M151
			MV04000HOT	D302	M151
			MV08000HOT	D302	M151
			MV01000DNL	D302	M151
			MV02000DNL	D302	M151
			MV03000DNL	D302	M151
			MV04000DNL	D302	M151
			MV08000DNL	D302	M151

*Special counties:

- 48201 (Harris)
- 48339 (Montgomery)
- 48157 (Fort Bend)
- 48291 (Liberty)
- 48071 (Chambers)
- 48167 (Galveston)
- 48039 (Brazoria)
- 48473 (Waller)
- 48085 (Collin)
- 48113 (Dallas)
- 48121 (Denton)
- 48439 (Tarrant)

GRDEM

The GRDEM module of EPS2x performs spatial allocation, or gridding. GRDEM was run to produce model-ready (UAM format) emissions files from the LBASE outputs. This module was also run with the PREAM outputs as input to spatially allocate the nonlink-based emissions. Spatial allocation surrogates were developed and applied to specific emission categories in accordance with NCTCOG documentation. The surrogates used and their applications are summarized in Table 2-7.

Table 2-7. Surrogates used to spatially allocate nonlink-based emissions.

Surrogate	Applicable emissions category
Zone area	Zone-based core county emissions (i.e. hotsoak, diurnal, local road)
Urban roadway	Perimeter county emissions associated with urban areas (as reported by NCTCOG)
Rural roadway	Perimeter county emissions associated with rural areas (as reported by NCTCOG)
County area	All others (i.e. emissions that NCTCOG did not spatially allocate)

Note that emissions from perimeter counties were distinguished between urban and rural by NCTCOG and so were delineated as such by using an extra tier in the ASCs. For instance, urban LDGV exhaust was assigned the ASC MV01210EXH. These detailed ASCs continued to have the speciation profile assigned to the higher-tier ASC (for instance, MV01210EXH used the same speciation profile as MV01000EXH) according to Table 2-6.

MRGUAM

The final step in the process stream involved merging the various pieces of each scenario's inventory into a single on-road emissions file. MRGUAM was used to combine the perimeter/core counties and link-/zone-based emissions.

3. PHOTOCHEMICAL MODELING

The Dallas/Fort-Worth (DFW) area was selected for photochemical modeling because of the relatively high contribution of on-road mobile source emissions in DFW compared to the Houston area. The importance of mobile source to ozone formation in DFW is expected to provide a clear indication of impacts of changing the methodology for spatially allocating hot soak and diurnal evaporative emissions.

The current Texas State Implementation Plan (SIP) for ozone in DFW is based on modeling completed by the TCEQ for ozone episodes in 1995 and 1996 (TNRCC, 2000). The TCEQ is currently developing a new DFW episode for August 1999, but the new episode is not yet completed. The existing June 18-22, 1995 episode was the basis for this study.

The DFW June 1995 photochemical modeling databases are set-up with a 32/16/4 km nested-grid structure, as shown in Figure 3-1. The 32 km grid covers a large regional domain to capture any ozone contributions from regional or long-range transport. The 12 km nested grid covers eastern Texas to better describe the regional contributions to ozone from areas immediately upwind. The 4 km nested fine-grid covers the DFW nonattainment counties at high resolution to accurately describe ozone formation in the DFW area. The TCEQ modeled the base year (1995) using CAMx (ENVIRON, 2003) and completed a model performance evaluation. Then, the TCEQ evaluated emission reduction strategies for a 2007 future year and completed a 1-hour ozone attainment demonstration (TNRCC, 2000). This modeling is based on the 2007 attainment demonstration scenario.

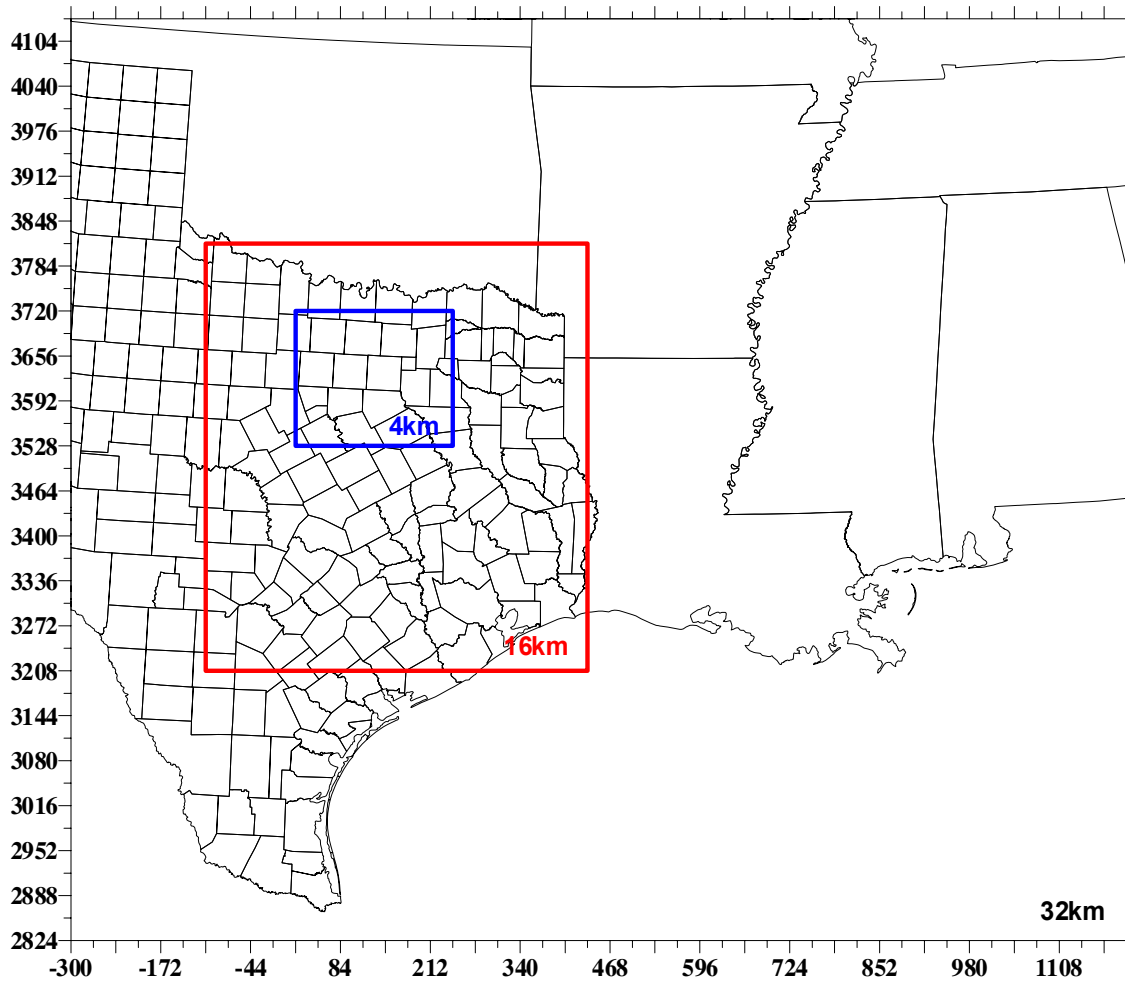


Figure 3-1. Dallas-Fort Worth (DFW) 32/16/4-km nested grid structure used in the June 18-22, 1995 SIP modeling episode.

The TCEQ developed the modeling inputs as described in the SIP documentation (TNRCC, 2000) and summarized below.

- Meteorology is from the SAI mesoscale model (SAIMM). The SAIMM is a relatively simple prognostic meteorological model that is no longer being used for air quality studies in Texas. However, the TCEQ was able to obtain acceptable ozone model performance with the SAIMM meteorology, in part because SAIMM has four-dimensional data assimilation (4DDA) to nudge the modeled meteorology toward the observed data.
- Boundary and initial conditions. The TCEQ developed initial and boundary conditions from available observational data. These do not play a major role in the modeling because of the large regional modeling domain and adequate spin-up period.

The TCEQ used CAMx version 2.03 for the SIP modeling (TNRCC, 2000) because this was the current version of CAMx at the time the SIP was developed. For this study, we used the latest public-release of CAMx, which is version 4.02 (ENVIRON, 2003). A sample CAMx control file for one of the model runs for this study is shown in Figure 3-2. This control file documents the input files and options that were used.

The modified on-road mobile source emission inventories described in Section 2 were substituted into and evaluated using the TCEQ's June 18-22, 1995 SIP modeling database for DFW. The 2007 area/off-road, point, and biogenic emissions were unchanged across all scenarios. The modeled ozone and precursor concentrations were compared with the standard and refined mobile source emissions to determine the spatially and temporally resolved impacts on ozone and their relationship to the precursor emission changes. The impact on peak ozone levels was also examined to evaluate how the inventory changes would impact the ozone attainment demonstration.

```

Model Version      |VERSION4.0
Run Message       |DFW 2007: 950622 strat30 task0
Root output name  |/disk42/HARC/Spatial/CAMx/outputs/task0/camx.950622.task0
Start yr/mo/dy/hr |1995 06 22 0000.
End yr/mo/dy/hr   |1995 06 22 2400.
DT:max,in,emis,out|15. 60. 60. 60.
nx,ny,nz         |47 41 8
Coordinate ID     |UTM
xorg,yorg,dx,dy  |-300. 2824. 32. 32. 15
Time Zone        |6
PiG Parameters    |2000. 12.
Avg Output Species|23
                 |NO          NO2          O3          OLE          PAN          NXOY
                 |PAR          TOL          XYL          FORM         ALD2         ETH
                 |CRES         MGLY         OPEN         PNA          CO           HONO
                 |H2O2        HNO3         ISOP         MEOH         ETOH
Num fine nest     |2
il,i2,j1,j2,nz,mesh| 7 23 13 31 8 2
il,i2,j1,j2,nz,mesh|11 17 23 28 8 8
HoriAdv SMOLAR/BOTT|PPM
Chemistry solver  |CMC
Restart          |true
Chemistry        |true
Dry Deposition   |true
Wet Deposition   |false
PiG Submodel     |true
Staggered Winds |false
Treat Area Emiss|true
Treat Point Emiss|true
1-day Emiss Inputs|true
3-D average File |false
Source Apportion|false
Chemparam        |/models/camx/inputs/CAMx4.chemparam.3
Photolysis Rates |/inputs/common/camx_photorate.950618-950622.isop
Landuse          |/inputs/common/uamv_landuse.regional_32km_corrected
Height/Pressure  |/inputs/met/1995/uamv_zp.950622.regional_32km
Wind             |/inputs/met/1995/uamv_wind.950622.regional_32km.CAMx2
Temperature      |/inputs/met/1995/uamv_temp.950622.regional_32km.CAMx2
Water Vapor      |/inputs/met/1995/uamv_hum.950622.regional_32km
Cloud/Rain       |
Vertical Diffusivity|/inputs/met/1995/uamv_kv.950622.regional_32km
Initial Conditions|
Boundary Conditions|/inputs/bc-ic-tc/uamv_bc.950622.obs2
Top Concentration|/inputs/bc-ic-tc/uamv_tc.yymmdd.clean
Albedo/Haze/Ozone|/inputs/common/uamv_aho.950618-950622.regional_32km+etx_16km+dfw_04km_58x50
Point Emiss      |/inputs/emiss/uamv_el_ei.950622.2007d.tier2_07Midlo50Nwr
Area Emiss       |/inputs/emiss/emiss.all.dfw_sip.32km.950622.base07
Landuse          Grid#1 |/inputs/common/uamv_landuse.etx_16km
Landuse          Grid#2 |/inputs/common/uamv_landuse.dfw_04km_58x50
Hght/Press      Grid#1 |/inputs/met/1995/uamv_zp.950622.etx_16km
Hght/Press      Grid#2 |/inputs/met/1995/uamv_zp.950622.dfw_04km_58x50
Wind            Grid#1 |/inputs/met/1995/uamv_wind.950622.etx_16km.CAMx2
Wind            Grid#2 |/inputs/met/1995/uamv_wind.950622.dfw_04km_58x50_mix.CAMx2
Temperature     Grid#1 |/inputs/met/1995/camx_temp.950622.etx_16km.CAMx2
Temperature     Grid#2 |/inputs/met/1995/camx_temp.950622.dfw_04km_58x50.CAMx2
Water Vapor     Grid#1 |
Water Vapor     Grid#2 |
Cloud/Rain      Grid#1 |
Cloud/Rain      Grid#2 |
Vert Diff       Grid#1 |/inputs/met/1995/uamv_kv.950622.etx_16km
Vert Diff       Grid#2 |/inputs/met/1995/uamv_kv.950622.dfw_04km_58x50
Area Emiss      Grid#1 |/inputs/emiss/emiss.all.dfw_sip.16km.950622.base07
Area Emiss      Grid#2 |/disk42/HARC/Spatial/CAMx/inputs/task0/emiss.all.dfw_2007.4km.950622.strat30
Coarse grid restart|/disk42/HARC/Spatial/CAMx/outputs/task0/camx.950621.task0.inst.2
Fine grid restart|/disk42/HARC/Spatial/CAMx/outputs/task0/camx.950621.task0.finst.2
PiG restart     |/disk42/HARC/Spatial/CAMx/outputs/task0/camx.950621.task0.pig

```

Figure 3-2. Sample CAMx4 control file for the Dallas/Fort-Worth June 1995 episode.

4. RESULTS

Table 4-1 summarizes the on-road NO_x and VOC emissions in the MOBILE5- and MOBILE6-based inventories used by NCTCOG (1998) prepared for this work. These emissions represent the 37-county DFW modeling domain, delineated by DFW and perimeter county groupings.

Table 4-1. June 19 DFW (Dallas, Denton, Collin, Tarrant) and perimeter counties on-road emissions (tons per day) developed for use in this work.

Area Category	MOBILE5		MOBILE6	
	NO _x	VOC	NO _x	VOC
Core	147.4	72.7	135.4	65.7
Perimeter	125.6	51.3	148.8	30.9
Total	273.0	124.0	284.2	96.6

Note that the MOBILE5 emissions include an adjustment for Tier 2 emission standards and low sulfur fuel and that both inventories include the effects of controls corresponding to TCEQ's Strategy 30 control scenario (TNRCC, 2000). Even with the correction for Tier 2 effects for MOBILE5 results, MOBILE6 emissions are still lower overall for VOC and core county NO_x. Several possible explanations exist, including reduced deterioration rates and road type-specific emission rates in MOBILE6. The higher NO_x in the perimeter counties, which have higher percentage of travel due to HDDVs, may be due to off-cycle HDDV NO_x effects incorporated in MOBILE6. Finally, the diurnal and hotsoak portions constitute about 17 and 25% of the above VOC totals for MOBILE5 and MOBILE6, respectively.

Figures 4-1a through d show the gridded on-road VOC emissions with zone-based and link-based spatial-allocation schemes as estimated by MOBILE5 and MOBILE6. As expected, for each allocation scheme, the MOBILE6 inventories have lower emission concentration peaks (due to lower overall emissions). On the other hand, it seems counterintuitive that there are higher emission concentration peaks (i.e. within results for the same model) in the zone-based scenarios, especially in Dallas County. However, an examination of the size of TAZs relative to a grid cell and the spatial distribution of zone-based emissions revealed the possibility that summing zone-based emissions and then redistributing them based upon links can have the net effect of dispersing these emissions rather than concentrating them. Figure 4-2, which shows the distribution of zone-based hotsoak emissions for TOD 13 (5 to 6pm) on June 19, illustrates how these emissions which are originally concentrated in a handful of TAZs would be dispersed when distributed onto travel network links (represented in Figure 4-3). This result may be specific to the travel demand modeling for the DFW area (in particular, to the way TAZs are defined) and might not occur for other areas.

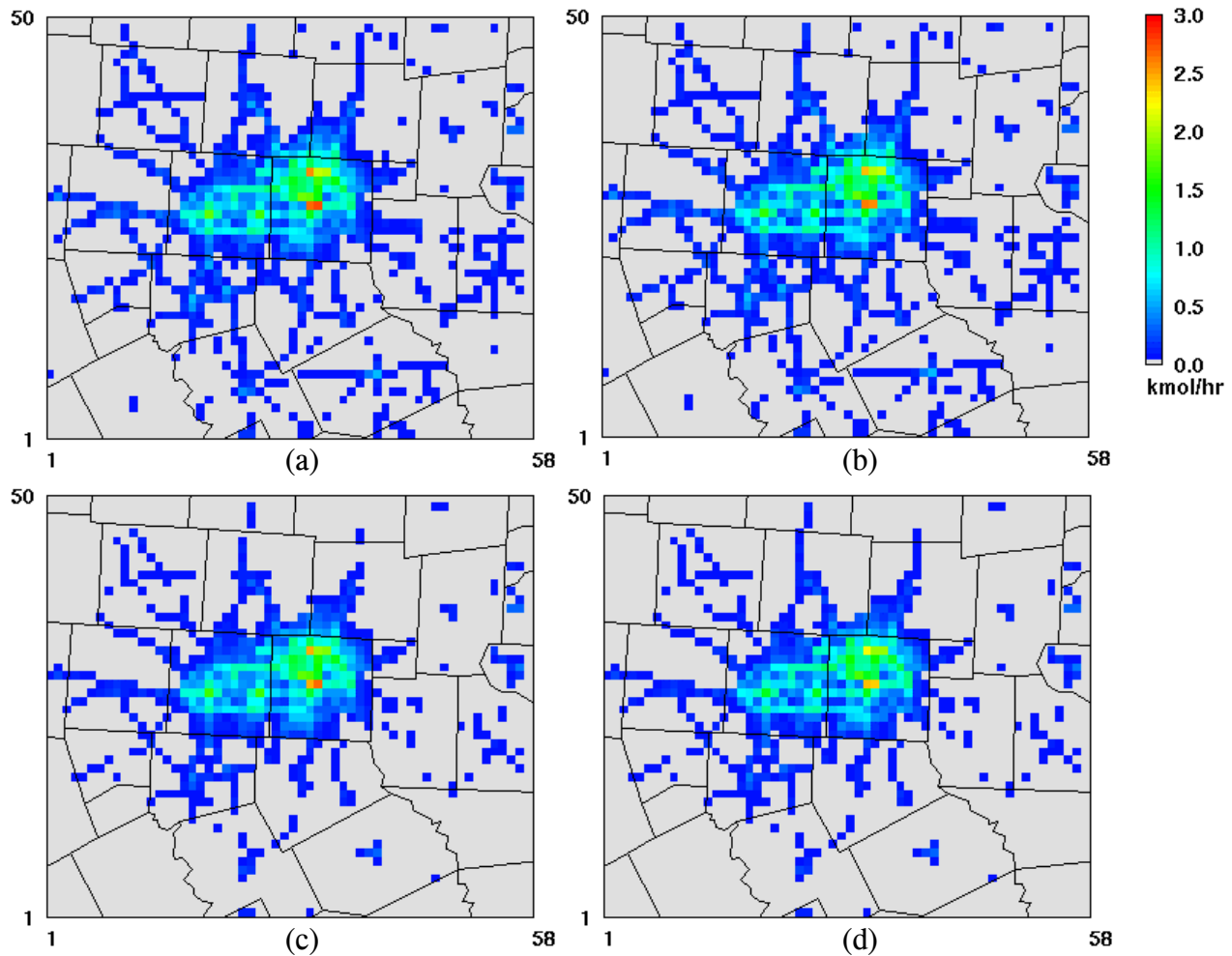


Figure 4-1. On-road mobile source emissions with hotsoak and diurnal VOC allocated based on zones (MOBILE5 (a); MOBILE6 (c)) and based on links (MOBILE5 (b); MOBILE6 (d)) at 16:00 on June 19.

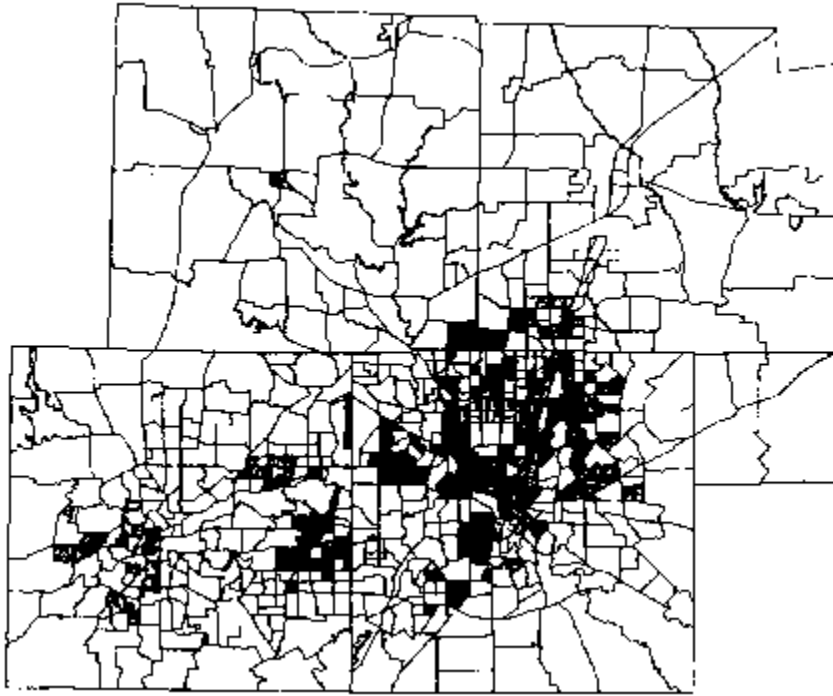


Figure 4-2. Distribution of zone-based hotsoak emissions within the core counties for TOD 13 of June 19th. (Taken from Exhibit II-3.5 of [NCTCOG, 1998]).

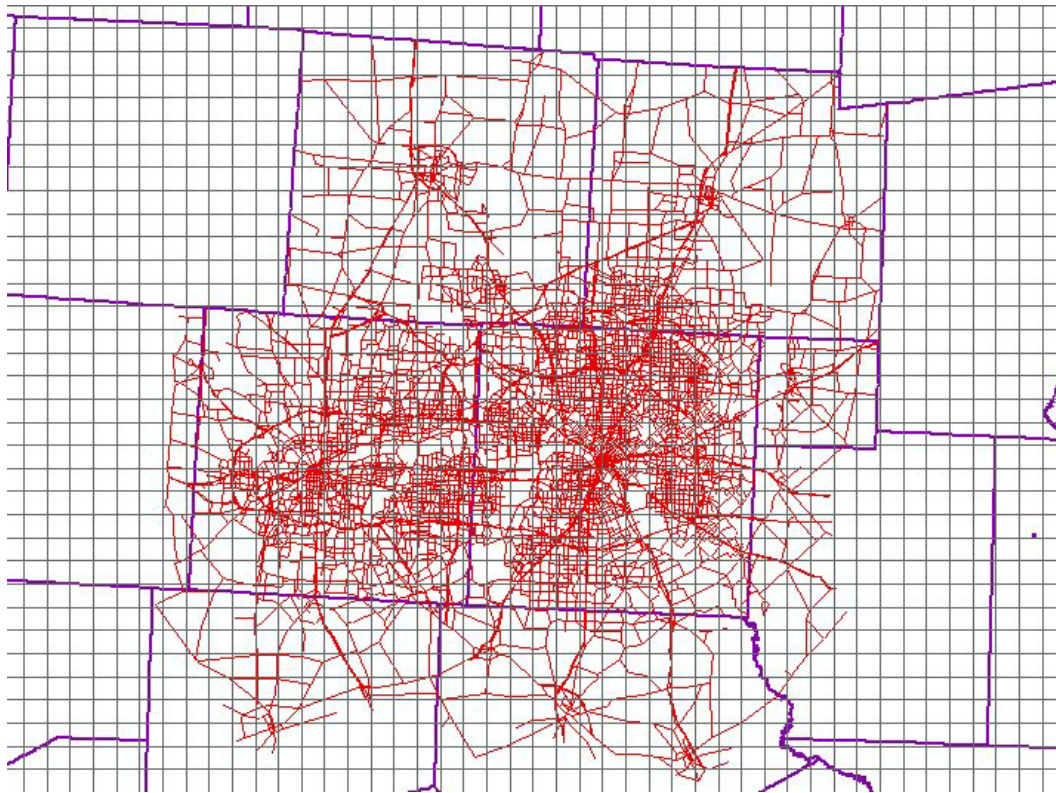


Figure 4-3. DFW transportation network used as the basis for allocating hotsoak and diurnal emissions using link-based VMT.

Figures 4-4a and b show the difference in predicted ozone concentrations between the zone-based and link-based emission scenarios for MOBILE5- and MOBILE6-based emissions, respectively. These figures are at the time of the largest absolute differences within the entire episode and occurred during the 16th hour on June 19th and represent the upper bound of the modeled impacts.

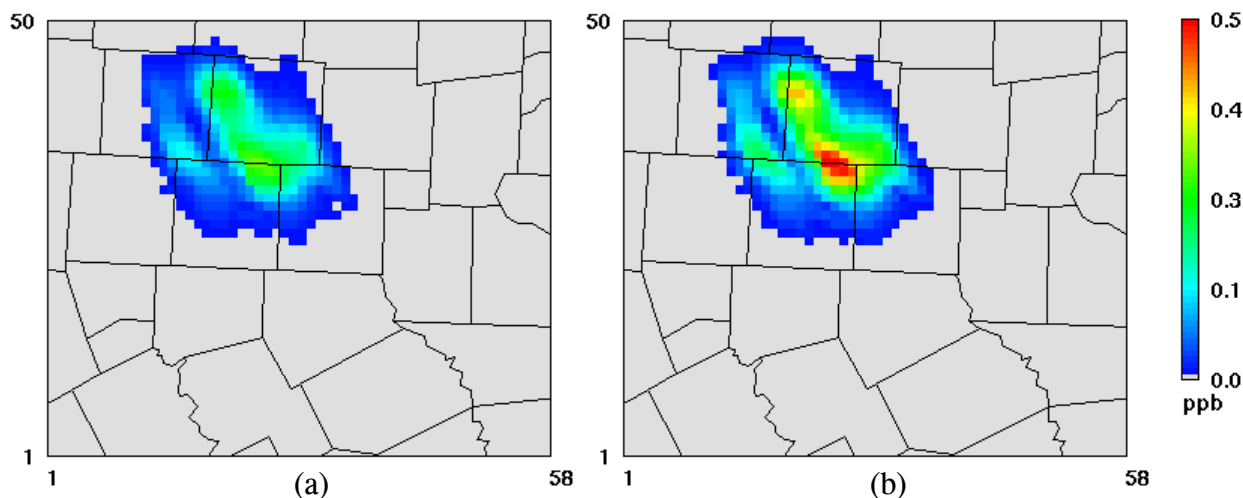


Figure 4-4. Increases in ozone due to link-based allocation of hotsoak and diurnal VOC emissions with MOBILE5 (a) and MOBILE6 (b) at 16:00 on June 19.

The first important observation is that the MOBILE6 scenario shows larger impacts of the spatial reallocation because the evaporative portion of the inventory is relatively larger in MOBILE6 than MOBILE5. Second, the magnitudes of these differences (<0.5 ppb) are minor when compared to the daily maximum concentrations (see Table 4-2). According to the table, the reallocation of the hotsoak and diurnal emissions did not significantly impact the daily maximum concentrations and, for the most part, did not affect the location of the observed maxima (i.e., except the for first day). Lastly, the episode's peak ozone also remained relatively unchanged (at ~124 ppb) for all scenarios. The most probable cause for these observed minor impacts is the fact that area/off-road and biogenic emissions together still dominate the VOC inventory. Figures 4-5a and b show the gridded on-road and area/nonroad VOC emissions for the hour corresponding to the differences observed in Figure 4-4 while Table 4-3 shows the contributions to VOC emissions on a daily, core county-wide basis.

Table 4-2. Modeled daily maximum ozone concentrations and their locations.

Scenario	Episode day	Maximum Ozone conc. (ppb)	Grid Cell Location
MOBILE5-based, zone-based	June 19 th	53.2	(19,39)
MOBILE5-based, link-based	June 19 th	53.3	(21,38)
MOBILE6-based, zone-based	June 19 th	53.5	(19,39)
MOBILE6-based, link-based	June 19 th	53.6	(21,38)
MOBILE5-based, zone-based	June 20 th	99.9	(27,37)
MOBILE5-based, link-based	June 20 th	99.9	(27,37)
MOBILE6-based, zone-based	June 20 th	99.5	(27,37)
MOBILE6-based, link-based	June 20 th	99.4	(27,37)

Scenario	Episode day	Maximum Ozone conc. (ppb)	Grid Cell Location
MOBILE5-based, zone-based	June 21 st	114.8	(30,33)
MOBILE5-based, link-based	June 21 st	114.7	(30,33)
MOBILE6-based, zone-based	June 21 st	115.1	(30,33)
MOBILE6-based, link-based	June 21 st	115.0	(30,33)
MOBILE5-based, zone-based	June 22 nd	123.9	(31,34)
MOBILE5-based, link-based	June 22 nd	123.8	(31,34)
MOBILE6-based, zone-based	June 22 nd	124.2	(31,34)
MOBILE6-based, link-based	June 22 nd	124.1	(31,34)

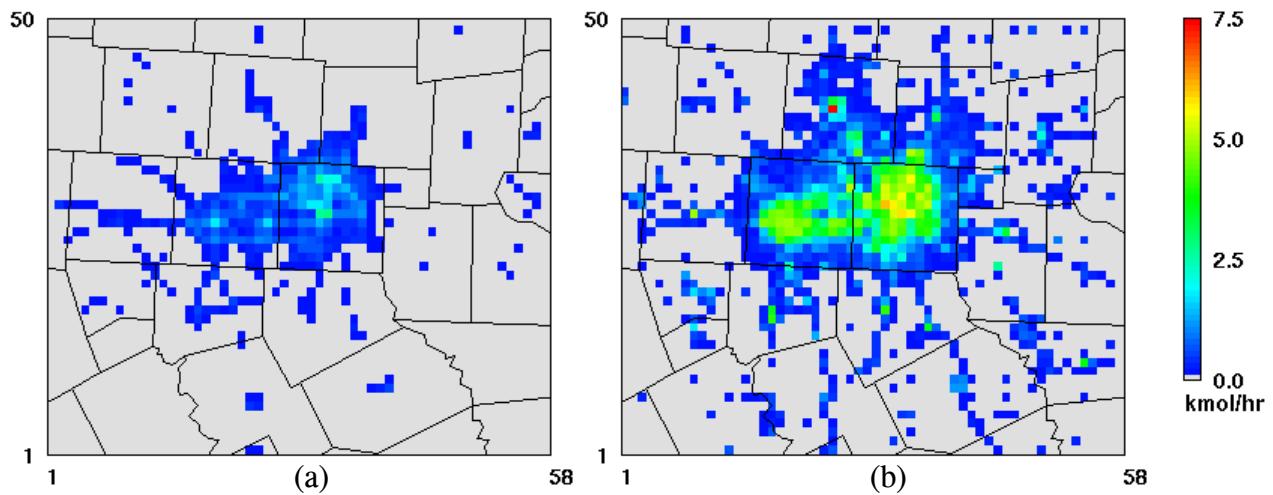


Figure 4-5. On-road mobile source (a) and area/non-road (b) emissions of VOC at 16:00 on June 19.

Table 4-3. Summary of VOC emissions contributions from 4 core counties in the Dallas-Fort Worth area on June 19.

Source Category	Contribution (%)	
	MOBILE5	MOBILE6
Mobile	14.5	13.4
Area/Off-Road	49.9	50.6
Points	2.8	2.8
Biogenic	32.8	33.2
Total	100.0	100.0

5. CONCLUSIONS

In this study, we made use of a pre-existing inventory where the hotsoak and diurnal evaporative emissions were spatially allocated using the TAZ-based approach. In general, however, this approach requires more effort and data for implementation than the link-based approach. The additional work may be justified by the magnitude of the effect upon predicted ozone, which depends upon three factors:

- the percent contribution of the relevant emission modes
- the relationship between TAZs and links, and
- the sensitivity of the area's ozone level to changes in VOC.

For the DFW area, whether MOBILE5 or 6 is used, the impact is relatively small (< 1ppb). (The impact is larger when MOBILE6 is used because of higher evaporative proportions.) This is consistent with the 2007 attainment demonstration in which these emissions constitute less than 20 percent of the VOC emissions even though DFW has a relatively high contribution from on-road sources. Another factor affecting these results is the size and proximity of hotsoak/diurnal zones in relation to a grid cell and to one another, respectively. If these zones are small and relatively concentrated (e.g. in downtown business districts) and the county does not have intersections of major freeways and arterials, using the link-based allocation may actually disperse these emissions. Such is the case for DFW. Therefore, these characteristics need to be reviewed before TAZs are used for allocation purposes. Lastly, VOC allocation changes are limited in effect by the area's sensitivity (i.e., is the region VOC-limited). Strongly VOC-sensitive areas would enhance the effect of allocation methodology.

Houston has some areas that are VOC-sensitive, but these do not necessarily coincide with a high contribution of mobile source emissions. Given the small impact seen in DFW and the high effort required for zone-based allocation, this approach should not be a high priority in Houston.

REFERENCES

- ENVIRON (2003). "User's Guide: Comprehensive Air Quality Model with Extensions (CAMx), Version 4.00." ENVIRON International Corporation, June 2003.
- ERG, (2001). Route56 input file translator software. Available at <http://www.ergweb.com/projects/mobile/index.htm>. ERG, Inc., February, 2001.
- NCTCOG (1998). "1995/96 & 1999 On-Road Mobile Source Episodic Emission Inventories for the Dallas-Fort Worth 37-County Modeling Domain." Transportation Department, North Central Texas Council of Governments, September 4, 1998.
- TCEQ (2003). Internal document summarizing how control scenarios were modeled. Provided to ENVIRON by TCEQ via ftp (file READ_ME.DFW_Growth_and_ControlZ). Texas Commission on Environmental Quality, July 1, 2003.
- TNRCC (2000). "Revisions To The State Implementation Plan (SIP) for the Control of Ozone Air Pollution, Dallas/Fort-Worth Attainment Demonstration." Texas Natural Resource Conservation Commission, April 19, 2000. Available from <http://www.tnrcc.state.tx.us/oprd/sips/apr2000dfw.html> (accessed August 11, 2003).