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MODEL SUITE TO ESTIMATE OZONE AND PM FROM FUEL REFORMULATION

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MODEL SUITE TO ESTIMATE OZONE AND PM FROM FUEL REFORMULATION

Final Report

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EXECUTIVE SUMMARY

Increased reformulated fuel use may impact emissions of criteria pollutants and criteria pollutant precursors and thus affect air quality. We present here updates to and applications of a modeling suite comprising the Consolidated Community Emissions Processing Tool (CONCEPT) and the Comprehensive Air Quality Model with Extensions (CAMx) to study the relationship between reformulated fuel use, on-road and non-road emissions, and ambient ozone and particulate matter (PM).

CONCEPT is an emission model that uses a database software technology (PostgreSQL) to calculate emission inputs for air quality modeling (Janssen and Wang, 2003; Loomis et al., 2005). The use of the database software makes CONCEPT a transparent model compared to the previous generation emission models. CONCEPT also offers the advantage of flexibility to the user in terms of quality control and performance; access to intermediate calculation steps facilitates quality control while providing useful transparency to the user. Different modules in CONCEPT predict emissions for different source categories such as area, point, mobile and biogenic sources. The on-road and non-road mobile source modules are the focus of this study.

The purpose of this work was to allow the use of data (external to the mobile source emissions models in CONCEPT) reflecting alternative fuel formulations or vehicle technology. The idea was to “simplify” and quicken the modeling of emissions and ozone and PM impacts due to the use of alternative fuel formulations.

The work presented here does not represent an effort to comprehensively simulate emissions and air quality impacts due to the use of alternative fuel formulation, but to demonstrate a “proof of performance” of this version of CONCEPT coupled with the air quality grid model CAMx. These results are not intended to be a comprehensive representation of alternative fuel impacts, rather a demonstration of the utility of the CONCEPT/CAMx model suite.

CONCEPT uses the EPA models, MOBILE and NONROAD, for the calculation of on-road and non-road emissions, respectively. The publicly available version of CONCEPT on-road is fully functional. However, the CONCEPT non-road module provided was incomplete. As part of the current study, we first completed the implementation of NONROAD version 2002 in CONCEPT. We modified the CONCEPT on-road and non-road modules to provide for flexibility in studying the effect of reformulated fuels and new technologies on on-road and non-road emissions. Resulting changes in ambient air quality were then predicted using the CAMx air quality model.

Figure E-1 shows the steps taken to develop and test flexibility for changes in fuel and technology types in the CONCEPT on-road mobile source emissions model. We modified CONCEPT v.0.71 to use the EPA standard version of MOBILE 6.2, with additional options to modify emission factors based on user inputs. Unlike the version of

MOBILE originally implemented in CONCEPT, the standard EPA version provides disaggregated emission factors for 25 model years and 28 vehicle types which enable us to more easily model the effect of alternative fuels and technologies.

A performance analysis of the CONCEPT on-road code revealed a bottleneck in a processing step that creates a table with MOBILE 6.2 output matched to the corresponding input definition for use in emission calculations. This was resolved by modifying the scripts to speed up processing (with negligible change in outputs) resulting in lower memory and CPU requirements. In step 3, alternative emission factors of conventional and reformulated gasoline were used to calculate adjustments to the emission factors of MOBILE6.2 for light-duty vehicles. The alternative emissions factors may be obtained from vehicle test programs or from models such as the California Reformulated Gasoline Phase 3 (CaRFG3) Predictive Model. In the case of the CA predictive model, the emission factors adjusted are those of exhaust and/or evaporative (diurnal, resting, hot soak and running) emissions of NO_x, HC, CO, benzene, 1,3-butadiene, formaldehyde, and acetaldehyde.

It should be noted that while models such as the CA predictive model exist to predict mass emissions from on-road vehicles, there are limitations in these models. Data on off-road engines and on speciation is more limited than data on vehicle mass emissions. Also, there is limited recent data on fuel effects on high emitters so fuel effects on high emitters are assumed to be the same as normal emitters. Fuel effect data on PM is more limited than data on HC, CO and NOx. In general, there have not been many evaluations of fuel effects on US vehicles in recent years so the underlying data to project fuel effects is very limited. Also, while vehicle technology changes can be accounted for by changes in emission factors in the modified CONCEPT, the application discussed here considers only fuel changes.

In step 4, CAMx simulations were conducted using emissions factors for conventional and reformulated gasoline in the Southeast Michigan Council of Governments (SEMCOG) network over a domain at 12 km resolution over the Upper Midwest for July 15-17, 2005. Other emissions and other inputs were obtained from the Lake Michigan Air Directors Consortium (LADCO) and were held constant between the base and alternative fuel scenarios.

NO_x emissions in the model showed a 3% increase on average across all on-road emissions categories due to 100% use of reformulated gasoline in light-duty vehicles in the SEMCOG network. There is a 13% decrease in CO emissions in the model across all categories. The CONCEPT on-road module simulates emissions of several volatile organic compounds (VOCs) including, for example, formaldehyde and ethanol. There is a 3% overall decrease in formaldehyde emissions predicted by CONCEPT due to the reformulated gasoline use with decreases in exhaust emissions and increases in evaporative emissions. Exhaust emissions of ethanol predicted by CONCEPT also decrease but larger increases in evaporative running and resting losses result in a 5% increase overall in ethanol emissions.

Very small changes in surface hourly ozone are predicted (decreases of up to 0.6 ppb in some areas and increases by up to 0.4 ppb in others) in and near southeastern Michigan due to the use of reformulated gasoline in the SEMCOG network. 8-hr surface ozone concentrations also decrease by less than 1 ppb and surface 24-hr average $PM_{2.5}$ concentrations decrease typically by less than 1.0%. Smaller increases in both pollutants are seen in some areas. The effect of reformulated gasoline on $PM_{2.5}$ is seen farther away from the SEMCOG area than that seen for ozone, reflecting, in part, the transport of PM precursors and secondary $PM_{2.5}$ formation.

The emissions and ozone/$PM_{2.5}$ results are presented here only to demonstrate the CONCEPT/CAMx model suite and should interpreted with caution because of limitations in the CA predictive model and because the CONCEPT/CAMx application is conducted here over a short time period of 3 days with limited data.

Differences in fuel properties among different types of fuels in US are decreasing and are much smaller that they were 10-15 years ago. With reductions in fuel sulfur there is now very little difference in sulfur content between conventional and reformulated fuels. Also ethanol blending continues to increase, there have been significant changes in the conventional gasoline over the past 5-10 years particularly in the amount of ethanol use. The use of ethanol will narrow differences in oxygenate, aromatics and distillation properties between conventional and reformulated fuels. Thus, the emissions and air quality impact of fuel differences modeled in the report (with and without 10% ethanol) are overestimated.

Figure E-2 shows a flowchart representing the steps taken to study the impact of alternative fuels and technologies in the CONCEPT non-road module (hereafter, CONCEPT-Nonroad). The NONROAD2002 code in CONCEPT-Nonroad reads emissions factors and outputs emissions. Hence, emission factors input to NONROAD2002 are modified to account for the effect of switching to a reformulated fuel unlike in the CONCEPT on-road module where emission factors output from MOBILE6.2 are modified. The emission factors in CONCEPT-Nonroad are specified for exhaust HC, CO, NO_x and PM and crankcase and diurnal HC emissions. The alternative fuel and technology module reads user-provided test and other data, where available, for technology types, deterioration factors and emission factors. The module updates the existing NONROAD2002 data files based on these data and processing is continued as before in CONCEPT.

In a test application, we updated the NONROAD2002 input data for emission factors for two categories of small two-stroke gasoline-powered handhelds, string trimmers and chainsaws, based on measurements conducted by the National Exposure Research Laboratory, U.S. EPA, and reported in the literature for these two categories when operated with conventional gasoline and 10% ethanol blend (E10). These data were used in CONCEPT-Nonroad for Texas (only one state was chosen for processing for this demonstration). All other states used the default fuel in CONCEPT-Nonroad. Non-road emissions of VOCs such as acetaldehyde and higher aldehydes, ethene and olefins decrease approximately by up to 0.4% in parts of Texas and non-road CO emissions decrease by up to 0.25% due to E10 use in trimmers and chainsaws. NO_x emissions show no noticeable change. $PM_{2.5}$ emissions decrease by up to 0.1% in isolated areas in Texas.

CAMx simulations were conducted over the central and eastern US at 36 km resolution domain using the CONCEPT-Nonroad emissions for conventional gasoline and E10 described above for July 15, 2005. New emission factors for the effect of ethanol on conventional gasoline were used only for string trimmers and chainsaws in Texas; other states used the conventional gasoline default emission factors in NONROAD2002. Other emissions data and other inputs were identical between the base and alternative fuel scenarios. A CAMx simulation was conducted for July 15, 2005 with initial conditions obtained from the last hour on July 14, 2005 of a prior annual CAMx simulation for 2005 available from LADCO. The small changes in non-road emissions result in a negligible change in hourly and 8-hour ozone. Small $PM_{2.5}$ impacts (decreases of up to 2% and increases of up to 4%) are seen in scattered areas in Texas and elsewhere due to transport. The results shown here are only from a sample simulation to demonstrate that the CONCEPT output can be easily interfaced with CAMx and should not be generalized.

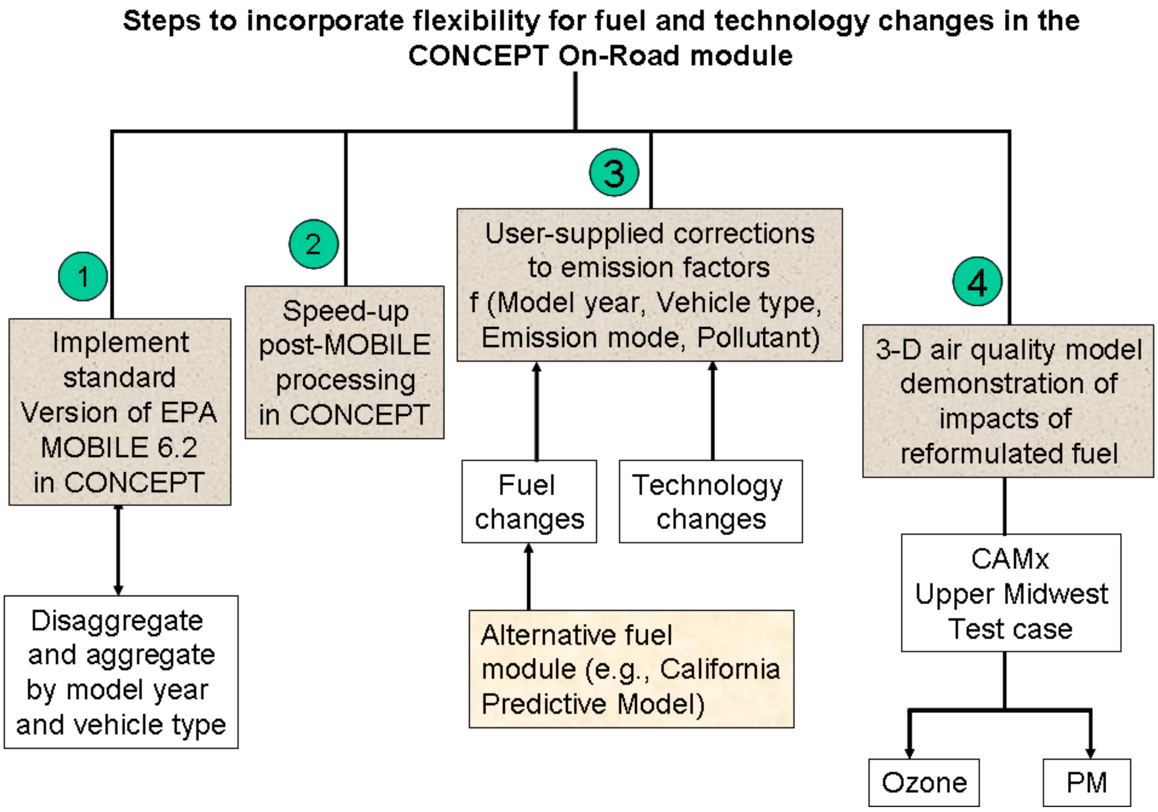

Figure E-1. Flexibility for reformulated fuel and technology changes in the CONCEPT on-road mobile source emissions model.

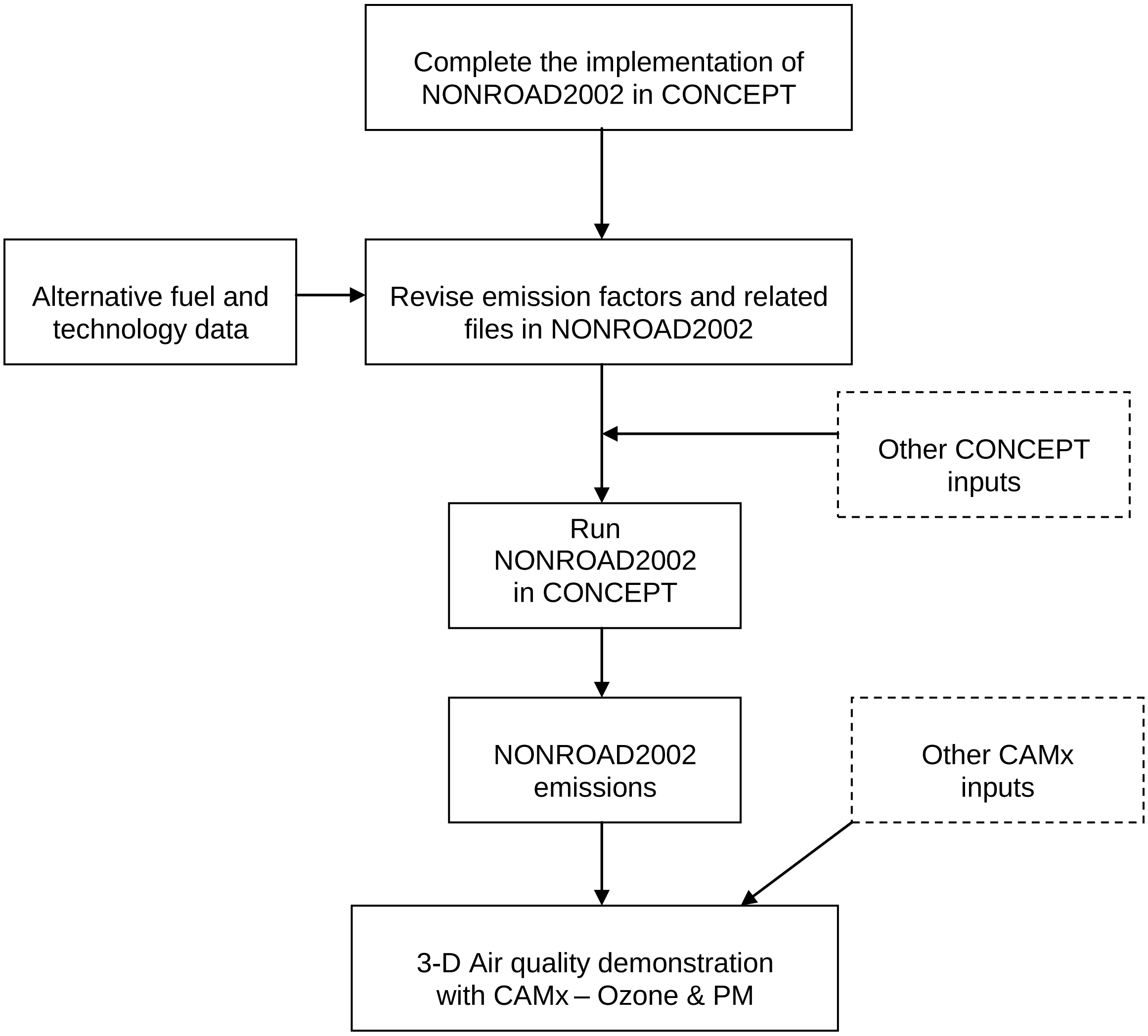

Figure E-2. CONCEPT non-road emissions processing steps.

1. INTRODUCTION

Emissions from mobile sources – on-road and non-road – affect the ambient concentrations of ozone, particulate matter (PM) and some air toxics. Those mobile source emissions depend on the fuels being used and the technology implemented to control emissions. The on-road vehicle fleet includes a variety of vehicles using different fuels and emission control technology depending on vehicle class and model year. Similarly, non-road vehicles and engines use different fuels and incorporate different technology types. It is desirable to be able to assess the effect of different fuels and emission control technology on air quality under realistic conditions, i.e., taking into account newer developments in fuel use and emission control technology.

The Consolidated Community Emissions Processing Tool (CONCEPT) is an emission model that uses a database software technology (PostgreSQL) to calculate emission inputs for air quality modeling (Janssen and Wang, 2003; Loomis et al., 2005). CONCEPT uses Structured Query Language (SQL) scripts to perform a majority of the emissions calculations. In addition, shell scripts and Perl scripts are also used within CONCEPT to interface between different modules (e.g., initiation, area, point, on-road mobile, non-road, speciation, output) and control several executables that are integrated within CONCEPT. The use of the PostgreSQL database and scripting languages makes CONCEPT a transparent model compared to the previous generation emission models. Intermediate data can be stored within the PostgreSQL and expert SQL users can query for quality assurance (QA) purposes. Scripts are also available to perform some standard QA and summary steps.

Currently, the mobile source emission module of CONCEPT uses MOBILE and NONROAD for the calculation of on-road and non-road emissions, respectively, based on fuel and vehicle fleet/non-road engine inputs. It offers some flexibility to address the effect of various transportation control measures that pertain to traffic activity, but it does not allow the user to make changes regarding fuel usage and the implementation of new emission control technology by vehicle class, model year and roadway type or by engine type and year. The overall objective of this study is to improve the mobile source emission module of CONCEPT to offer the desired flexibility to investigate how reformulated fuels and emission control technology scenarios influence emissions from on-road and non-road vehicles and equipment. Subsequent changes in ambient ozone and PM concentrations are then predicted using the Comprehensive Air Quality Model with Extensions (CAMx), an advanced 3-D Eulerian model (Morris et al., 2003). CONCEPT and CAMx together comprise the model suite discussed in this study.

Section 2 presents the modifications made to the CONCEPT on-road module to provide for flexibility in studying alternative fuels and technologies and a study of air quality impacts using a CAMx test case. In Section 3, we explain our procedure for incorporating NONROAD2002 in CONCEPT and discuss the modifications to the CONCEPT-Nonroad module for implementing new fuel and technology data and a related CAMx test case. Section 4 provides a summary of this study.

2. MODIFICATIONS TO THE CONCEPT ON-ROAD MOBILE SOURCE MODULE

2.1. Overview of CONCEPT-Mobile

A flow chart representing the current on-road mobile source module in CONCEPT (hereafter referred to as CONCEPT-Mobile) is shown in Figure 2-1. A key feature of CONCEPT-Mobile is the incorporation of a modified version of EPA's MOBILE 6.2 (http://www.epa.gov/OTAQ/m6.htm), which is an emission factor model for predicting gram per mile emissions of hydrocarbons (HC), carbon monoxide (CO), nitrogen oxides (NO_x), carbon dioxide (CO_2), PM, and toxics from cars, trucks, and motorcycles under various conditions. MOBILE 6.2 is written in FORTRAN. CONCEPT prepares input files for MOBILE 6.2 runs for combinations of (1) representative counties, (2) temperatures, (3) calendar years, (4) seasons, and (5) speed. The MOBILE 6.2 executable is executed using a shell script. For each combination, the output contains entries for 8 vehicle classes, 10 emission types, 5 road (facility) types, and 24 hours of the day. The CONCEPT-Mobile module currently employs a modified version of the standard version of MOBILE 6.2 from EPA to aggregate emissions from various model years and detailed vehicle types (28 vehicle types to 8 classes). MOBILE 6.2 outputs are loaded into the PostgreSQL database. Within the database, the MOBILE 6.2 factors are applied to specific pollutants from specific vehicle classes, emission modes and facility types based on activity data to generate emissions data.

2.2. Installing CONCEPT-Mobile

The source code (version 0.71) and a test case for CONCEPT-Mobile were obtained from the Lake Michigan Air Directors Consortium (LADCO) (M. Janssen, personal communication, 2009). Before running the code, a number of tools were installed. Instructions are found on the conceptmodel.org website and followed for PostgreSQL, PostGIS, PROJ.4, GEOS, and Perl. Based on our initial tests, the configuration of PostgreSQL is particularly important. Default PostgreSQL configurations are modified to maximize the resources allocated to only a few users. In other words, PostgreSQL resources cannot be shared among multiple CONCEPT runs and/or other users. Some key settings are as follows (S. Edick, personal communication, 2008):

max_connections = 10 (default =100)
shared_buffer = 128 MB (default = 8.2MB)
work_mem = 512 MB (default = 1 MB)
maintenance_work_mem = 512 MB (default = 16 MB)
max_fsm_pages = 256000 (default = 16000)
fsync = off (default = on)

Note that turning on fsync ensures that updates to the database are written to the hard disk. This increases the input/output (I/O) requirements, but allows the recovery of the database in a consistent state in case of an operating system or hardware crash. For a database with a large volume of data that cannot be easily recreated, the "off" setting may be risky. For CONCEPT, the database contents are either loaded from input files or calculated, thus can be recreated. With changes in the configuration of PostgreSQL, some memory settings of the Linux operating system have to be set accordingly.

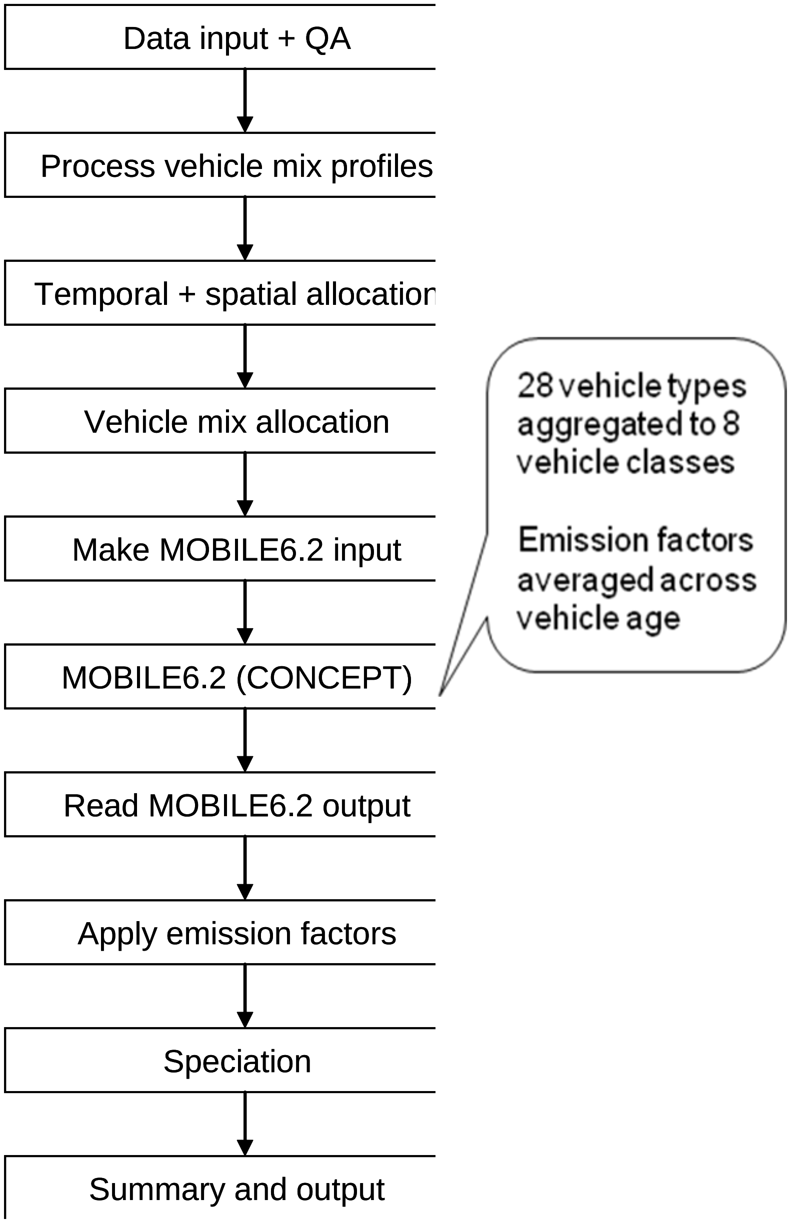

Figure 2-1. Flow chart representing the current CONCEPT-Mobile module.

CONCEPT-Mobile is a fairly resource-intensive model. It is preferable to employ machines with state-of-the art processors (> 2 GHz) with at least 4 GB of memory. Performance deterioration is noticeable on machines that have slower processors and less memory. Ample disk space is needed, especially for a new domain or new simulation where intermediate data are saved for QA purposes. For example, a CONCEPT-Mobile run generates over 10 GB of intermediate data for two days for the Southeastern Michigan Council of Governments (SEMCOG) network.

2.3. Testing and Speeding up CONCEPT-Mobile

A performance analysis of the CONCEPT-Mobile code revealed a bottleneck in a processing step that creates a table with MOBILE 6.2 output matched to the corresponding input definition for use in emission calculations. This step took 14 hours out of the total of 16 hours to run CONCEPT-Mobile and represented a prime candidate for possible speed-up. The resource-intensive SQL command in this step involves a "INSERT INTO ... SELECT ... FROM ...WHERE" construction and resides in a loop that is called for each hour, each pollutant, and each emission mode. The "INSERT INTO" part of the SQL statement populates a new temporary table with information from other tables. Information from those other tables is extracted using the "SELECT" statement. In one example, various fields are extracted from 5 tables. When multiple tables are involved, they are first joined together within the database before conditions are applied to prune the resulting entries. Out of the joined tables, entries representing matching rows from individual tables are kept. The reason why this type of SQL command is computationally expensive is that if the first table contains r1 rows and the second table contains r2 rows, the resulting joined internal table contains $r1 \times r2$ rows. Therefore, the number of rows grows in a combinatorial manner with the joining of multiple tables. In this example, the five tables being joined together contains 240952, 8, 14, 881280, and 771480 rows, respectively (maximum size of combined internal table is 1.8×10^{19} rows).

Instead of joining 5 tables in one SQL statement, a time saving solution is to break the command into two steps. The first step joins the first 4 tables (240952, 8, 14, 881280 rows, respectively), and selects the appropriate entries to be stored in a temporary table. The second step joins the temporary table (5.8×10^{6} rows) with the fifth table (771480 rows) and extracts data based on the equivalent criteria of the original statement. The maximum sizes of the two intermediate tables are 2.4×10^{13} and 4.5×10^{12} rows, respectively. The smaller, more easily manipulated tables are a key reason for the observed speed up.

As discussed above, the computationally intensive SELECT statement resides within a loop and is repeated many times. It is also realized that the first step of the streamlined approach, which matches 4 tables related to the conditions specified in the MOBILE 6.2 input file, can be consolidated so that it is run just once instead of once every hour for each combination of pollutant and emission mode. Storing the results for one of the joins results in extra disk space requirements while CONCEPT-Mobile is running. However, for the loop, joined tables are 6-7 orders of magnitude smaller. This results in lower memory and CPU requirements.

This faster version is used as the framework for development in this project.

A major difference between the MOBILE 6.2 model implemented within CONCEPT-Mobile and the standard EPA version of MOBILE 6.2 is the aggregation of 28 MOBILE 6.2 vehicle types into 8 classes. The CONCEPT-Mobile version also by default aggregates all model years (age), and omits lead as a pollutant. (Although refueling emission factors are provided by MOBILE 6.2, CONCEPT-Mobile does not estimate refueling emissions, but instead assumes that such emissions are included in the area or point source inventories.)

We downloaded the EPA standard version of MOBILE 6.2 from http://www.epa.gov/OTAQ/m6.htm. Because one of the objectives of this project is to provide full flexibility of the MOBILE model within CONCEPT, the standard version of MOBILE 6.2 was incorporated into CONCEPT. To understand the requirements for MOBILE 6.2 to work seamlessly with CONCEPT, we compared the input and output of the CONCEPT-Mobile version and the standard version of MOBILE 6.2.

As indicated in the CONCEPT User's Guide (Environ, 2005), the CONCEPT-Mobile version of MOBILE 6.2 requires an input file that specifies "DATABASE GROUPS." This part of the CONCEPT.IN input file, which is generated from a Perl script in CONCEPT, is excerpted as follows:

```
DATABASE GROUPS     : 8
                    : HDDV    11111 11111111 1 111 22222222 122
                    : HDGV    11111 22222222 1 111 11111111 211
                    : LDDT    11111 11111111 1 122 11111111 111
                    : LDDV    11111 11111111 1 211 11111111 111
                    : LDGT1   12211 11111111 1 111 11111111 111
                    : LDGT2   11122 11111111 1 111 11111111 111
                    : LDGV    21111 11111111 1 111 11111111 111
                    : MC      11111 11111111 2 111 11111111 111
```

These DATABASE GROUPS are specified in a manner quite similar to the input specification using DATABASE VEHICLES in the standard version of MOBILE 6.2. In CONCEPT-Mobile, MOBILE 6.2 is run 8 times with the various groupings, and the results are aggregated for all model years for each vehicle group. Detailed results can be achieved using the standard version by invoking the DATABASE YEARS command and specifying individual vehicle types using the DATABASE VEHICLES feature.

Several test cases were performed using the MOBILE 6.2 executable distributed with CONCEPT-Mobile and the standard version. The DATABASE output from MOBILE 6.2 provides emission factors to 4 decimal points. The CONCEPT-Mobile and standard versions sometimes differ in the last digit in the output. The CONCEPT-Mobile version has also been modified to suppress output when the emission factors are zero or below some threshold.

2.4. Modifying CONCEPT to use the Standard Version of MOBILE 6.2

The version of MOBILE 6.2 in the current CONCEPT-Mobile generates outputs that are aggregated into 8 vehicle classes and across model years. As discussed in Section 2.3, the standard EPA version of MOBILE 6.2 was installed instead in CONCEPT to take advantage of the detailed outputs by model years and by vehicle types. Some more detail on the procedure followed is described in this section.

The CONCEPT-Mobile version of MOBILE 6.2 was removed from CONCEPT and the standard version was inserted in the manner illustrated in Figure 2-2. Here, colored boxes represent changes to the original CONCEPT code; bold boxes represent new procedures added. CONCEPT is modified to write the input file for the standard version of MOBILE 6.2 as described in Section 2.3. Then, the MOBILE 6.2 executable is executed. Compared to the current CONCEPT-Mobile version, a detailed standard MOBILE 6.2 will produce approximately 85 times the volume of output, because MOBILE 6.2 disaggregates each emission factor into values for 25 model years and 8 vehicle classes into 28 individual types. To keep the output file size manageable, input files to run the standard version of MOBILE 6.2 are created for one vehicle type at a time (28 runs total). Also, the speed-up described in Section 2.3 is used to decrease computational time.

The processing of detailed standard MOBILE 6.2 output into the CONCEPT format is implemented outside of MOBILE 6.2 to provide the functionality to CONCEPT to modify the detailed emission factors based on user-defined technology or fuel effects. More information on the revision of emission factors is provided in Section 2.5. Following the revision of emission factors, a Perl script is used to reproduce the aggregation calculations performed within the CONCEPT-Mobile version of MOBILE 6.2. Perl is a language designed for processing text, and it is ideal for tasks involving the formatting and aggregating of large volumes of data. Perl is already used in CONCEPT to interface with MOBILE 6.2. It can be easily understood by CONCEPT users who are familiar with shell and SQL scripts.

Two separate steps are performed. The first step is to calculate the aggregate emission factor (EF in g/mi or g/start) for all model years.

$$\left\langle EF \right\rangle^{yr} = \sum_{iyr} \frac{RD_{iyr} \cdot VMT_{iyr}}{\sum_{jyr} (RD_{jyr} \cdot VMT_{jyr})} \cdot EF_{iyr}$$

where the terms on the right hand side are as follows: iyr and jyr refer to individual years, RD is the registration distribution of vehicles for the year, VMT is the miles travelled, and EF is the emission factor for the vehicle for the year. Therefore for each vehicle type, the aggregated emission factor is a weighted average of emission factors for vehicles of different model years. This step is performed for each vehicle type, and this is the point where post standard MOBILE 6.2 modifications to emission factors of specific model year of individual vehicle types can be applied.

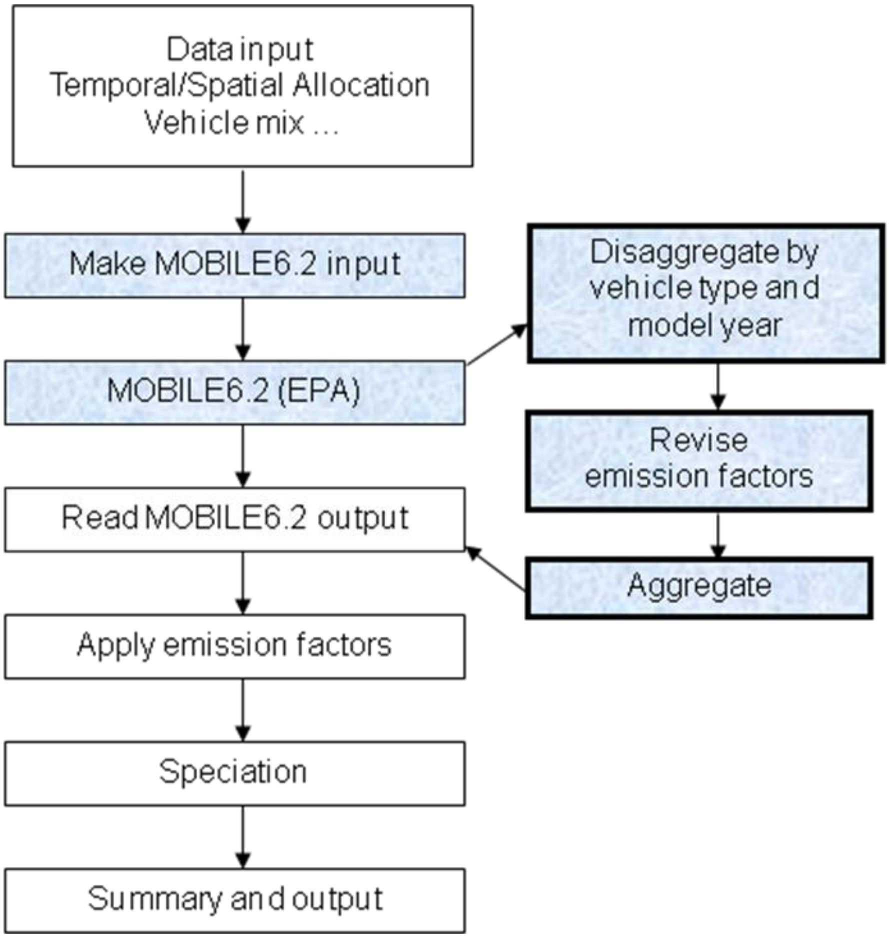

Figure 2-2. Flow chart representing the on-road mobile source module in CONCEPT, modified to use the EPA standard version of MOBILE 6.2. Colored boxes represent changes to the original CONCEPT code; bold boxes represent new procedures added.

In the second step, 28 vehicle types are aggregated into 8 vehicle classes. Several vehicle classes contain only one vehicle type: LDDV, LDGV, and MC. Of the remaining classes, HDDV contains 10 MOBILE 6.2 vehicle types, HDGV contains 9 vehicle types, and LDDT, LDGT1, and LDGT2 contain two vehicle types each. The emission factor for each class is a weighted average based on the fraction of each vehicle type belonging to that vehicle class:

$$EF_{v\_class} = \sum_{itype} \frac{Count_{itype} \cdot VMT_{itype}}{\sum_{jtype} (Count_{jtype} \cdot VMT_{jtype})} \cdot EF_{itype}$$

where the terms on the right hand side are as follows: itype and jtype refer to individual vehicle types, Count is the number in the given type and VMT is the miles travelled in the given type. Different subscripts itype and jtype are used for individual vehicle types to reflect the fact that summing is first done in the denominator over all vehicle types (jtype) and then the sum is used as the denominator for the overall ratio that is again summed over all vehicle types (itype).

Detailed standard version MOBILE 6.2 results processed using the Perl scripts are fed back into CONCEPT. Any difference in the final emission output files generated using these results, as opposed to the CONCEPT-Mobile version of MOBILE 6.2, can be traced back to the last significant digit in the output files of standard MOBILE 6.2 output files.

As discussed above, the large volume of raw data from MOBILE 6.2 necessitated a code design to run MOBILE 6.2 for each vehicle type. In addition, resources for input and output (I/O) also became a significant issue for the Perl processing step. To optimize the CONCEPT code, MOBILE 6.2 output was streamlined to contain only variables that are used in subsequent CONCEPT calculations. The original format of the database output from MOBILE is shown below; and fields that are suppressed in the output are struck through.

(1) file number
(2) run number
(3) scenario number
(4) pollutant
(5) vehicle type
(6) emission type
(7) facility type
(8) age
(9) hour
(10) EF in gram per mile
(11) EF in gram per hour
(12) number of engine starts
(13) trip ends
(14) miles
~~(15) miles per gallon~~
~~(16) hour VMT %~~
~~(17) facility VMT %~~
(18) registration distribution
(19) vehicle count
~~(20) ambient temperature~~
~~(21) diurnal temperature~~
~~(22) model year~~

Many of these suppressed output variables are echoed from MOBILE 6.2 inputs and are not calculated by MOBILE 6.2. Therefore, there is no loss of information by eliminating them from the standard MOBILE 6.2 output.

2.5. Modification of Emission Factors to Account for Reformulated Fuels and Alternative Technologies

As discussed above, the CONCEPT-Mobile on-road vehicle module is modified to use the EPA standard version of MOBILE 6.2, with additional options to modify emission factors based on technology and fuel changes. Unlike the current CONCEPT-Mobile version of MOBILE 6.2, the EPA standard version provides disaggregated emission factors for 25 model years and 28 vehicle types which enable us to more easily model the effect of alternative fuels and technologies. Perl code is used to apply adjustment factors to the MOBILE 6.2 emission factors and to aggregate those factors and convert them to CONCEPT post-processor-ready format. A separate input text file is used by the user to specify adjustment factors. This file contains fields of vehicle class, emission type, and pollutant number, followed by 25 fields of emission adjustment factors for 25 model years (age). If no adjustment factor is specified for a given combination of vehicle type, emission type, and pollutant number, no adjustment will be applied to the standard MOBILE 6.2 output for that combination.

While the modified CONCEPT can accept alternative emission factors from any source (e.g., vehicle test programs), here the California Reformulated Gasoline Phase 3 (CaRFG3) Predictive Model (*http://www.arb.ca.gov/fuels/gasoline/premodel/premodel.htm*) is used here as an example to provide alternative emission factors that are used to calculate the adjustment factors discussed above. The California Predictive Model is a spreadsheet-based model used to determine compliance of alternative gasoline formulations with California Cleaner-Burning Gasoline regulations. We use the Phase 3 for PM Flat for Producers version 12-31-09 of the CaRFG3 predictive model (pmproducers2007.xls). This spreadsheet is based on procedures defined by ARB for evaluating alternative specifications for Phase 3 reformulated gasoline (ARB, 2008).

It should be noted that while models such as the CA predictive model exist to predict mass emissions from on-road vehicles, there are limitations in these models. Data on off-road engines and on speciation is more limited than data on vehicle mass emissions. Also, there is limited recent data on fuel effects on high emitters so fuel effects on high emitters are assumed to be the same as normal emitters. Fuel effect data on PM is more limited than data on HC, CO and NOx. In general, there have not been many evaluations of fuel effects on US vehicles in recent years so the underlying data to project fuel effects is very limited. Also, while vehicle technology changes can be accounted for by changes in emission factors in the modified CONCEPT, the application discussed here considers only fuel changes.

Table 2-1 shows the fuel properties for Phase 3 reformulated gasoline that need to be input to the California Predictive Model to evaluate these gasoline specifications as alternatives. The California Predictive Model consists of a number of sub-models (ARB, 2008). The sub-models are equations relating gasoline properties to the exhaust and evaporative emissions changes resulting from motor vehicle use. Table 2-2 shows the pollutants whose emissions are calculated by the California Predictive Model along with the respective emission modes. Twenty-one separate exhaust sub-models are available for seven pollutants (NO_x, HC, CO, benzene, 1,3-butadiene, formaldehyde, and acetaldehyde). Three exhaust sub-models are available for each of the seven pollutants: one sub-model for each of three vehicle emissions control technology "Tech" classes (Tech 3 (model years 1981-1985), Tech 4 (model years 1986-1995), and Tech 5 (model years 1996+)). In addition, six sub-models are available for evaporative emissions (ARB, 2008). Three sub-models are used for evaporative hydrocarbon emissions and three sub-models are used for evaporative benzene emissions. For both evaporative hydrocarbon emissions and evaporative benzene emissions, one sub-model is used for each of the following evaporative emission processes: 1) Diurnal/Resting Losses, 2) Hot Soak Emissions, and 3) Running Losses. Also, the evaporative processes include permeation emissions when ethanol is used.

Table 2-1. Properties for Phase 3 reformulated gasoline input to the California Predictive Model (source: ARB, 2008).

Fuel Property	**Units**
Reid vapor pressure (RVP)	psi
Sulfur (SUL)	ppmw
Benzene (BENZ)	vol.%
Aromatic hydrocarbons (AROM)	vol.%
Olefin (OLE)	vol.%
Oxygen (OXY) min.	wt. %
Oxygen (OXY) max.	wt. %
Temperature at 50 % distilled (T50)	deg. F
Temperature at 90 % distilled (T90)	deg. F

Table 2-2. California Predictive Model pollutants and corresponding units of measurement and emission modes (source: ARB, 2008).

Pollutant	**Units**	**Emission Mode**
Nitrogen oxides (NO_x)	g/mile	Exhaust
Carbon monoxide (CO)	g/mile	Exhaust
Hydrocarbons (HC)	g/mile	Exhaust
Hydrocarbons (HC)	g/mile	Evaporative
Benzene (BENZ)	mg/mile	Exhaust
Benzene (BENZ)	mg/mile	Evaporative
1,3-butadiene	mg/mile	Exhaust
formaldehyde	mg/mile	Exhaust
acetaldehyde	mg/mile	Exhaust

Figure 2-3 shows the steps associated with the modification of emission factors for alternative fuels and technologies. The base and alternative fuel properties are provided by the user. For testing, we use typical fuel properties of conventional and reformulated gasoline. The fuel properties specified in Table 1 are input to the California Predictive Model and the Predictive Model results are subsequently input to a script that creates an ASCII file with the format specified in Figure 2-4. Changes in the relevant emission factors are calculated by running the Predictive Model twice, first with the properties of the base fuel and then with the new (alternative or candidate) fuel.

The base fuel properties input to the California Predictive Model code are mapped to the fuel properties required by CONCEPT. In particular, E200 and E300 (the percentage of vapor of the gasoline fuel at 200 F and 300 F) for the base fuel are estimated from the California Predictive Model T50 and T90 specifications using conversions found in EPA's gasoline complex model spreadsheet (*http://www.epa.gov/oms/rfg.htm*).

$$E200 = 147.91 - (0.49*T50)$$
$$E300 = 155.47 - (0.22*T90)$$

The base fuel properties are input to CONCEPT to obtain emission factors which are then adjusted using Perl code. The code also includes flexibility to handle emission factor corrections due to technology changes indicated by the user. Two steps are subsequently performed: (1) the aggregate emission factor for all 25 model years is calculated and (2) the 28 vehicle types are aggregated into 8 vehicle classes (as discussed above). The aggregated emission factors are then transferred back to CONCEPT for speciation.

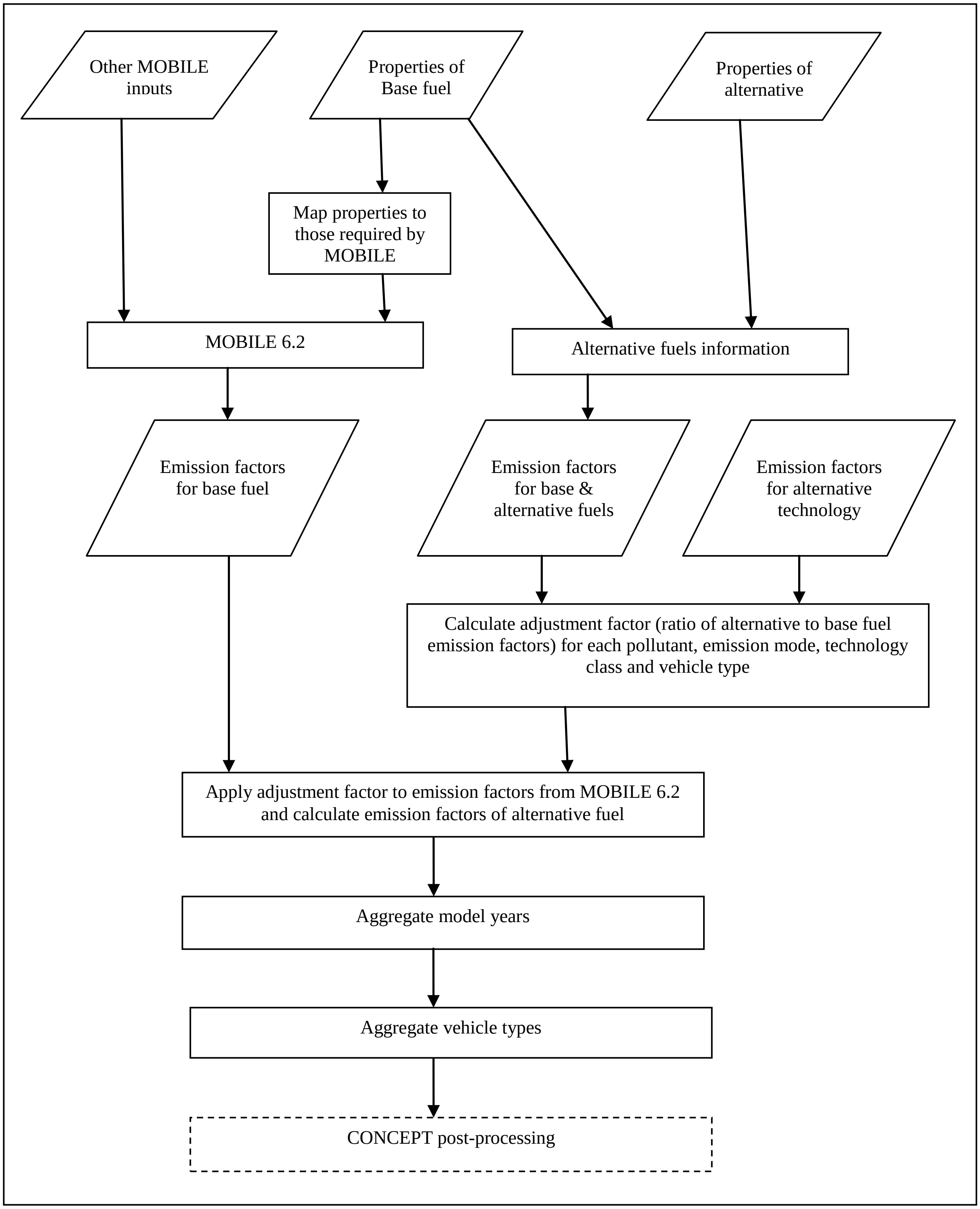

Figure 2-3. Flowchart of steps in the modification of emission factors for alternative fuels and technologies.

```
# Emission factors from California Predictive Model for exhaust and evaporative emissions for gasoline
# vehicles and trucks
#

# List of Tech Classes:
# Tech3  1981-1985  older closed-loop three-way catalyst
# Tech4  1986-1995  closed-loop three-way catalyst
# Tech5  1996+  three-way catalyst, adaptive learning, LEVs
#

# List of emission types:
# 1 Exhaust emissions from running operations
# 3 Evaporative emissions from hot soak
# 4 Evaporative emissions from diurnal conditions
# 5 Evaporative emissions from resting losses
# 6 Evaporative emissions from running losses
#

# List of pollutants (Mobile6.2 Pollutant#, Name and Units)
# 1 Hydrocarbons (HC)      g/mile
# 2 Carbon monoxide (CO)  g/mile
# 3 Nitrogen oxides (NOx)   g/mile
# 16 Benzene (BENZ)     mg/mile
# 18 1,3-Butadiene (BUTA) mg/mile
# 19 Formaldehyde (FORM)   mg/mile
# 20 Acetaldehyde (ACET)  mg/mile
# Note: Exhaust HC, CO, NOx, BENZ, BUTA, FORM and ACET and Evaporative HC and BENZ
#

# Fuel properties
Base fuel: RVP(psi), T50(F), T90(F), Arom(vol %), OLE(vol %), Oxygen_min(wt %), Oxygen_max(wt %),
Sulfur(ppmw), Benzene(vol %)
Alternative fuel: RVP(psi), T50(F), T90(F), Arom(vol %), OLE(vol %), Oxygen_min(wt %), Oxygen_max(wt
%), Sulfur(ppmw), Benzene(vol %)


# Emission Factors
Base_or_Alternative_Fuel, TechClass, EmissionType#, Pollutant#, Emission Factor
# Base fuel=1, Alternative fuel=2
1, 3,  1,  1,  0.15
 2, 3, 1,  1,  0.12
# …..…
```

Figure 2-4. Format of output from the script that reads emissions factors from the California Predictive Model.

2.6. Application of the Alternative Fuel Module

The alternative fuel module discussed above was tested in the SEMCOG network for July 15-17, 2005. The impact of using reformulated gasoline in this network on on-road mobile source emissions and air quality was analyzed as discussed below.

2.6.1. Impact of reformulated fuel use on on-road mobile source emissions

The properties of the base and alternative fuel applied to test the alternative fuel module in CONCEPT are shown in Table 2-3. These fuels correspond to conventional gasoline and Federal Reformulated Gasoline (RFG) (with ethanol) assumed for Detroit, Michigan in summer (AIR, 2005). Complete (100%) market penetration of the RFG is assumed in the test case. Changes have to be made to the code to handle partial market use. The T50 and T90 values of the RFG correspond to E200 and E300 values of 45% and 84%, respectively. Note that ethanol is prevalent in conventional gasoline in many parts of the country; the example provided is only to demonstrate the capabilities of CONCEPT and should be used with caution.

Table 2-3. Base and alternative fuel properties.

Fuel Property	**Units**	**Base Fuel (Conventional gasoline)**	**Alternative Fuel (Reformulated gasoline)**
Reid vapor pressure (RVP)	psi	6.9	6.8
Aromatic hydrocarbons (AROM)	vol.%	26.1	22.0
Benzene (BENZ)	vol.%	1.00	0.87
Ethanol (ETOH)	wt. %	0.0	3.5
Olefins (OLE)	vol.%	5.6	4.9
Sulfur (SUL)	ppmw	30	30
Temperature at 50 % distilled (T50)	deg. F	218	210
Temperature at 90 % distilled (T90)	deg. F	329	325

Figure 2-5 shows the distribution of on-road mobile source NO_x emissions by vehicle and emission type in the base fuel scenario in the SEMCOG network on July 16, 2005. Total on-road NO_x emissions in the SEMCOG area are 175 tons/day in the base fuel scenario. The two largest categories are exhaust emissions from heavy duty diesel vehicles (HDDVs) and light duty gasoline vehicles (LDGVs). Figure 2-6 shows the NO_x emissions from the top three gasoline-powered vehicle categories and the relative change in emissions in shifting from conventional gasoline to RFG. There is a 6% increase in NO_x emissions from these three categories and a 3% increase across all categories (not shown).

Figures 2-7 to 2-12 show similar plots for CO, formaldehyde (FORM) and ethanol (ETOH) emissions output from CONCEPT (FORM and ETOH are shown here as two examples of volatile organic compounds (VOCs)). Total CO emissions in the SEMCOG network are 1197 tons/day in the base fuel scenario. There is a large (>15%) and consistent decrease in CO emissions due to the use of the oxygenated fuel in the three categories (light duty trucks 1 and 2 and light duty gasoline vehicles) with the highest CO emissions. There is an 18% decrease in CO emissions from these three categories and 13% decrease across all categories. Exhaust FORM emissions show decreases of 5-6% due to RFG use while evaporative FORM emissions show increases of 1-14%. There is a 3% decrease overall in FORM emissions. Exhaust emissions of ETOH also decrease but the increases in evaporative running and resting losses more than compensate resulting in a 5% increase overall in ETOH emissions.

The emissions results presented here are only to serve as an example demonstration of the modified CONCEPT and should not be generalized because of limitations in the CA predictive model.

Differences in fuel properties among different types of fuels in US are decreasing and are much smaller that they were 10-15 years ago. With reductions in fuel sulfur there is now very little difference in sulfur content between conventional and reformulated fuels. Also ethanol blending continues to increase, there have been significant changes in the conventional gasoline over the past 5-10 years particularly in the amount of ethanol use. The use of ethanol will narrow differences in oxygenate, aromatics and distillation properties between conventional and reformulated fuels. Thus, the emissions and air quality impact of fuel differences modeled in the report (with and without 10% ethanol) are overestimated.

The computational time for the CONCEPT on-road module is 6 hours for one day in the SEMCOG network on a server with an AMD Opteron 290 2.8 GHz processor. The time indicated includes the last step of the CONCEPT processing, i.e., creation of the CAMx mobile source emissions file for SEMCOG (running CONCEPT for multiple networks would result in almost a linear increase in computational requirements). Prior to running CONCEPT, the alternative emission factors have to be obtained and provided in the format required and other CONCEPT inputs set up. The time required to set up CONCEPT is variable and depends mostly on the availability of alternative emission factors; it takes approximately 30 minutes if the emission factors are available. After the CONCEPT run, the CAMx emissions file created by CONCEPT for a given network (here SEMCOG) has to be merged with emissions from other networks to create the final CAMx-ready low-level emissions file. This process takes only a few minutes provided the other files are readily available. Overall, the effort required to use CONCEPT is mostly dictated by the actual CPU time of CONCEPT and not pre- or post-processing.

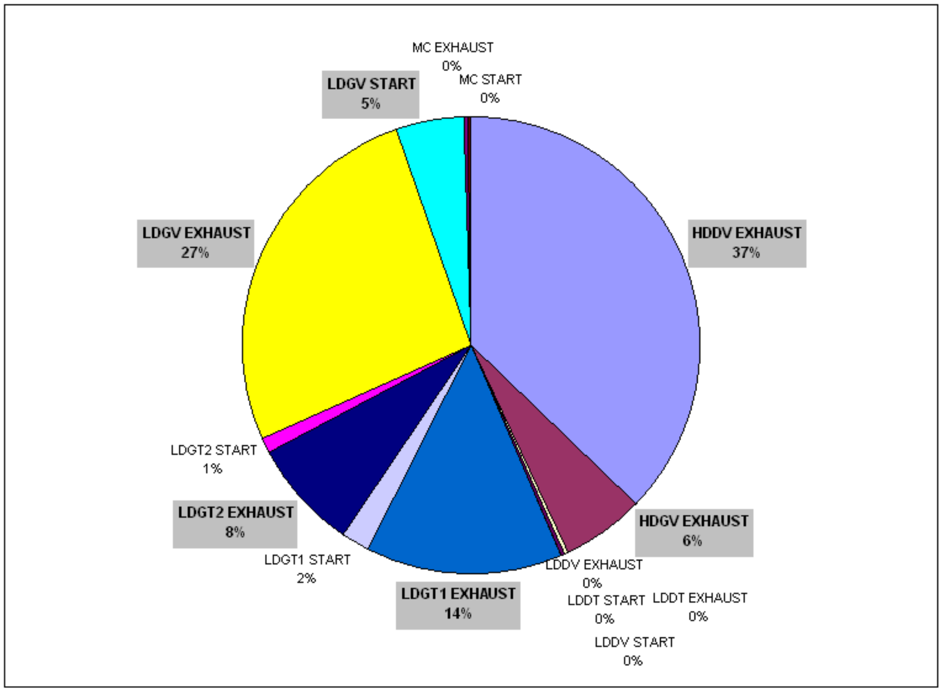

Figure 2-5. On-road NO_x emissions in the base fuel scenario in the SEMCOG network on July 16, 2005.

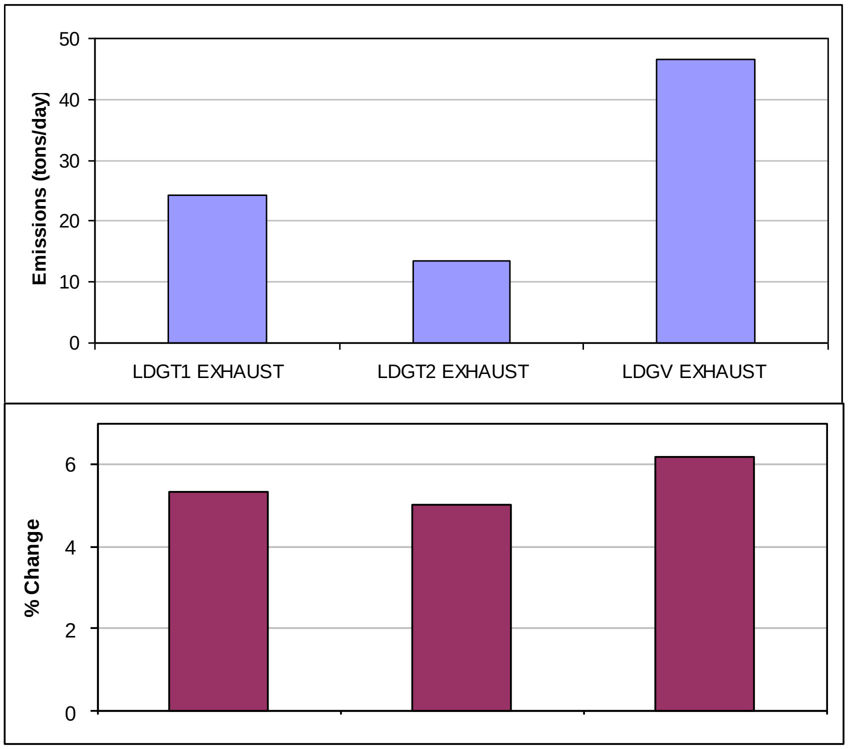

Figure 2-6. Effect of reformulated gasoline on on-road NO_x emissions in the model in the SEMCOG network on July 16, 2005; emissions due to conventional gasoline (top) and percent change due to reformulated gasoline (bottom).

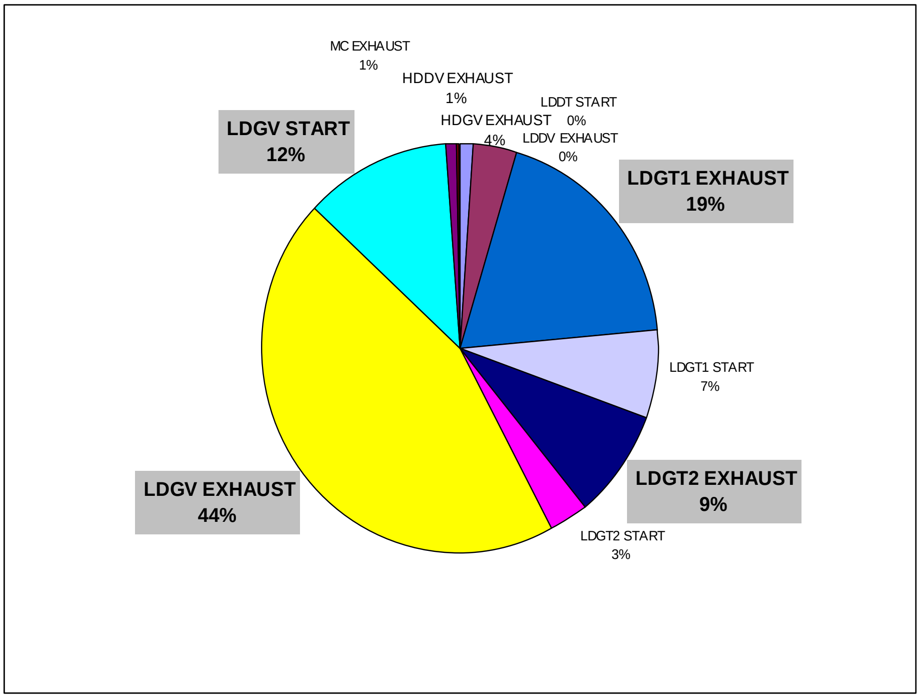

Figure 2-7. On-road CO emissions in the base fuel scenario in the SEMCOG network on July 16, 2005.

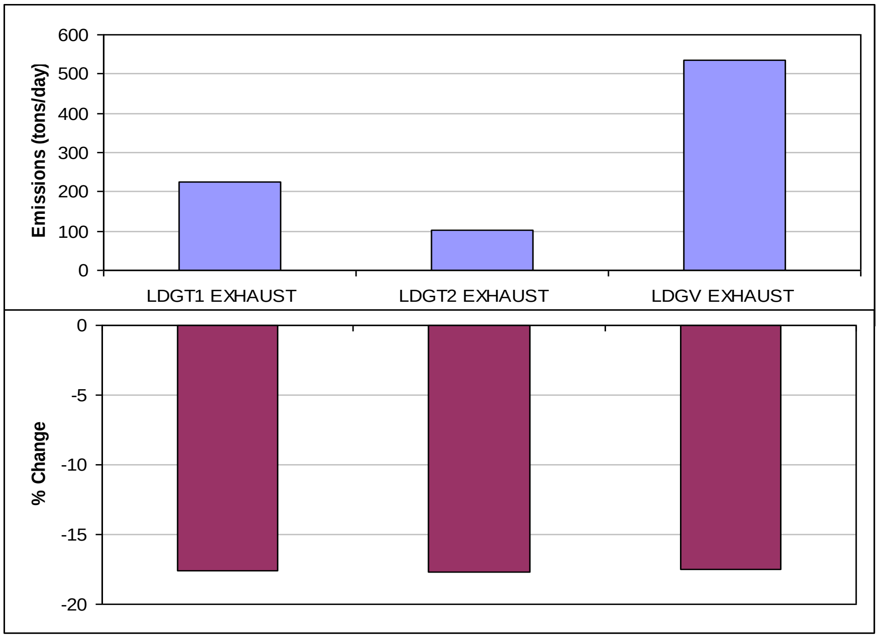

Figure 2-8. Effect of reformulated gasoline on on-road CO emissions in the model in the SEMCOG network on July 16, 2005; emissions due to conventional gasoline (top) and percent change due to reformulated gasoline (bottom).

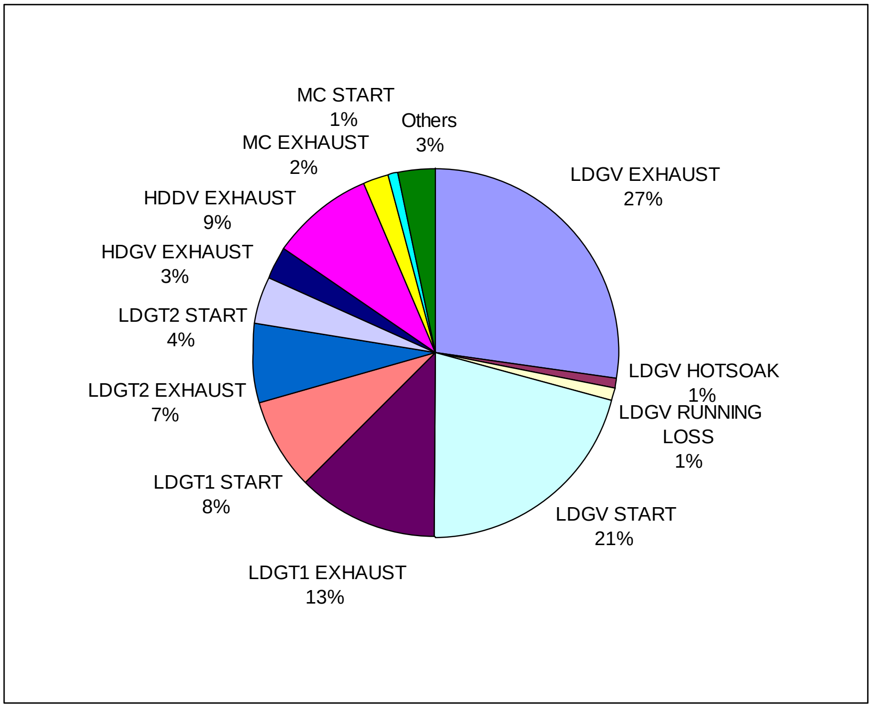

Figure 2-9. On-road FORM emissions in the base fuel scenario in the SEMCOG network on July 16, 2005.

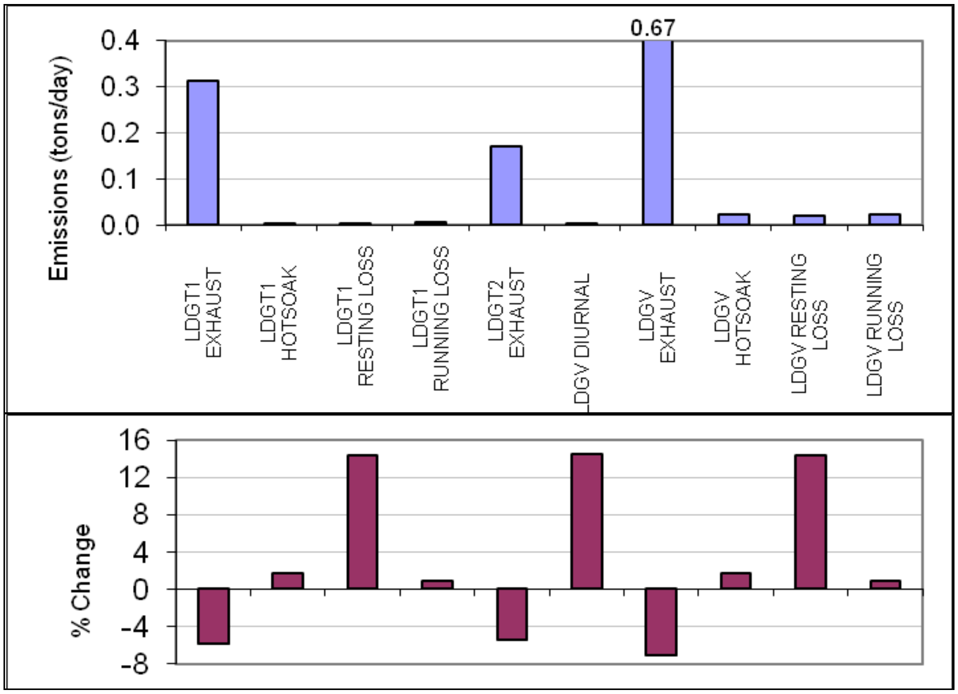

Figure 2-10. Effect of reformulated gasoline on on-road FORM emissions in the model in the SEMCOG network on July 16, 2005; emissions due to conventional gasoline (top) and percent change due to reformulated gasoline (bottom).

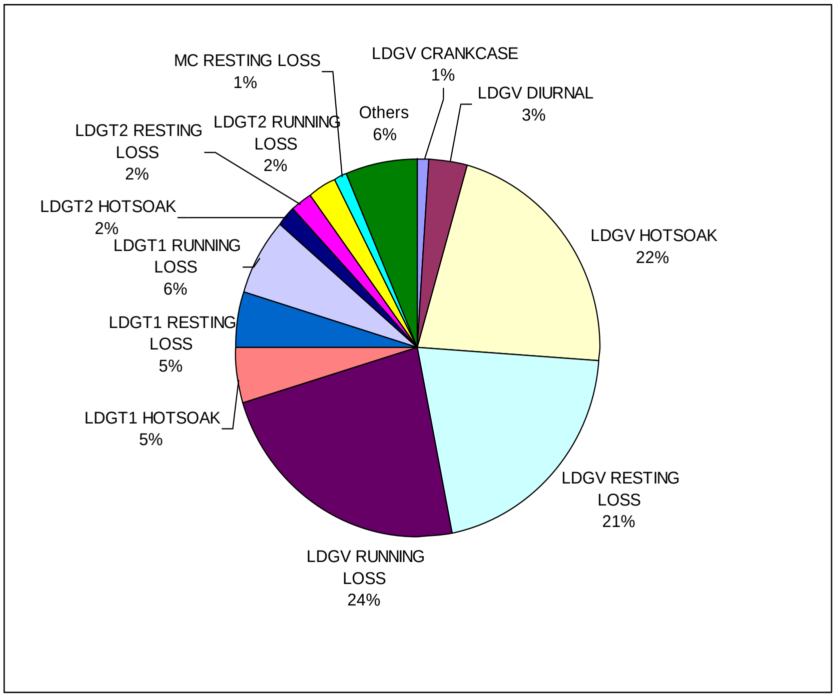

Figure 2-11. On-road ETOH emissions in the base fuel scenario in the SEMCOG network on July 16, 2005.

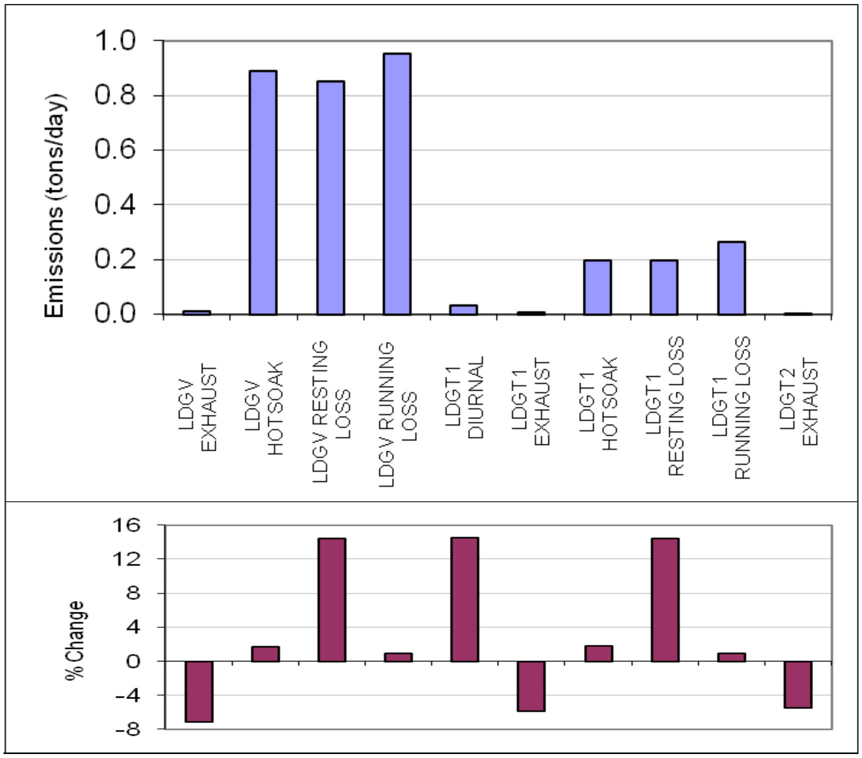

Figure 2-12. Effect of reformulated gasoline on on-road ETOH emissions in the SEMCOG network on July 16, 2005; emissions due to conventional gasoline (top) and percent change due to reformulated gasoline (bottom).

2.6.2. Impact of reformulated fuel use on ambient ozone and PM

CAMx simulations were conducted using the mobile emissions factors for conventional and reformulated gasoline in the SEMCOG network over a domain at 12 km resolution over the Midwestern US for July 15-17, 2005 (see inner domain in Figure 2-13). Other emissions data and other inputs were obtained from LADCO and were held constant between the base and alternative fuel scenarios. In particular, boundary conditions were obtained from a LADCO CAMx simulation at 36 km resolution (in the outer domain shown in Figure 2-13). The simulation results are described below. These results are not intended to be a comprehensive representation of alternative fuel impacts, rather a demonstration of the utility of the CONCEPT/CAMx model suite.

Figures 2-14 and 2-15 show the peak hourly surface ozone concentrations in the base fuel scenario on July 16, 2005 and July 17, 2005, respectively (July 15, 2005 is excluded from the analysis to partially account for the effect of not using model spin-up). Also shown are the changes in hourly surface ozone at the hour of maximum change due to use of reformulated gasoline in the SEMCOG network. Surface hourly ozone decreases by up to 0.6 ppb in some areas and increases by up to 0.4 ppb in others in the vicinity of the SEMCOG area. The ozone decreases and increases are due to changes in NO_x, VOC and CO emissions (depending on the region, ozone formation could be NO_x- or VOC-limited). CO contributes in small measure to ozone formation, although its reactivity is much lower than most of the VOC species.

It should be noted that the ozone and $PM_{2.5}$ results are presented here only to demonstrate the CONCEPT/CAMx model suite and should interpreted with caution because of limitations in the CA predictive model and because the CONCEPT/CAMx application is conducted here over a short time period with limited data. Also, emissions changes are not considered for non-road mobile sources, and non-light duty on-road sources. Also, other changes, such as area source refueling emissions, marketing and distribution, or ethanol production related emissions, are not included in this application.

Figures 2-16 to 2-19 show similar plots for 8-hr ozone (from noon to 7 pm EDT) and for 24-hr average $PM_{2.5}$ concentrations. 8-hr ozone changes by less than 1 ppb. Surface 24-hr average $PM_{2.5}$ concentrations change typically by less than 1.0%. The effect of reformulated gasoline is seen not only in Michigan but also in other Midwestern states, reflecting, in part, the transport of PM precursors and secondary $PM_{2.5}$ formation.

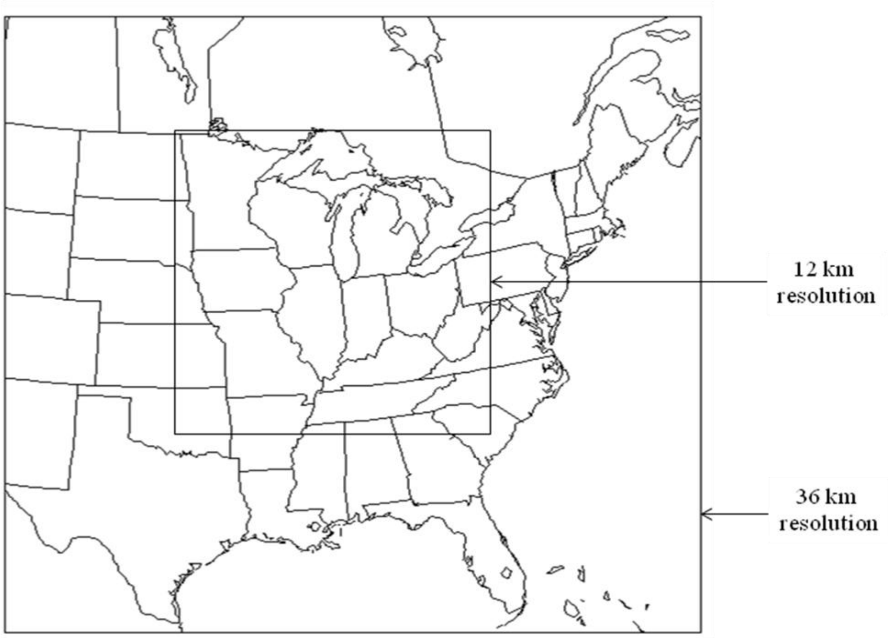

Figure 2-13. Nested domains at 36 km and 12 km resolutions for 2005 modeling.

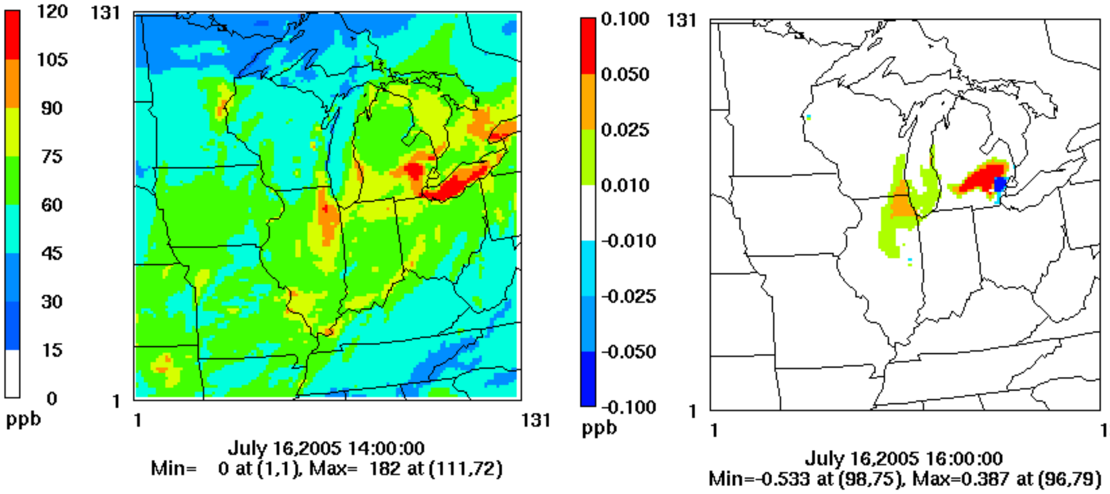

Figure 2-14. Impact of reformulated gasoline use in the SEMCOG network on surface ozone concentrations; peak hourly ozone concentration due to conventional gasoline (left) and change in hourly ozone at hour of maximum change due to reformulated gasoline (right) on July 16, 2005.

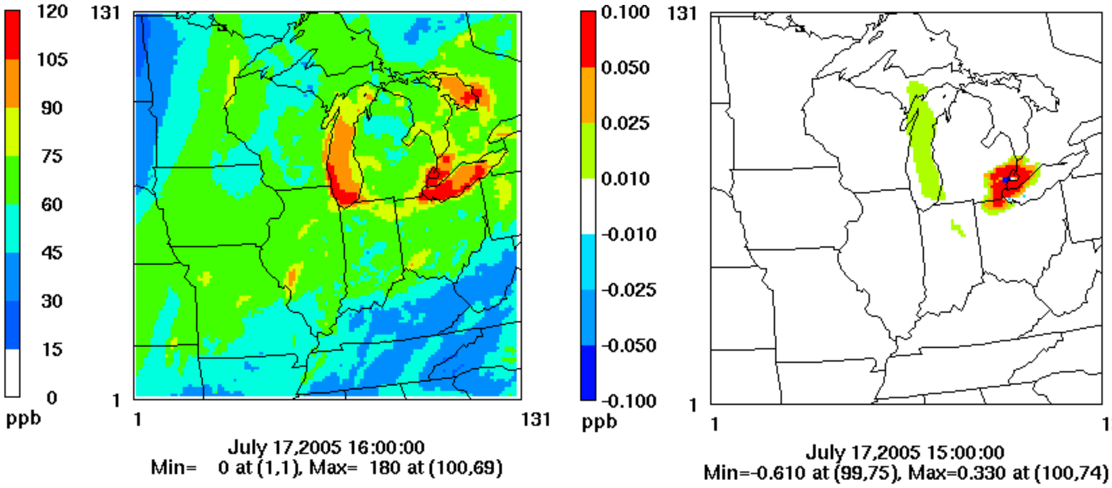

Figure 2-15. Impact of reformulated gasoline use in the SEMCOG network on surface ozone concentrations; peak hourly ozone concentration due to conventional gasoline (left) and change in hourly ozone at hour of maximum change due to reformulated gasoline (right) on July 17, 2005.

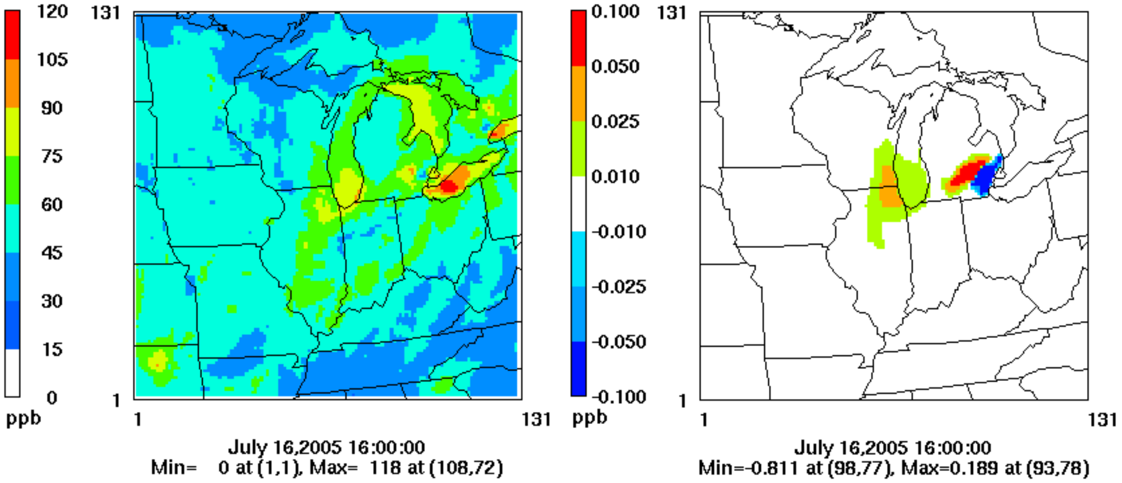

Figure 2-16. Impact of reformulated gasoline use in the SEMCOG network on surface ozone concentrations; 8-hour average (noon-7 PM EDT) ozone concentration due to conventional gasoline (left) and change due to reformulated gasoline (right) on July 16, 2005.

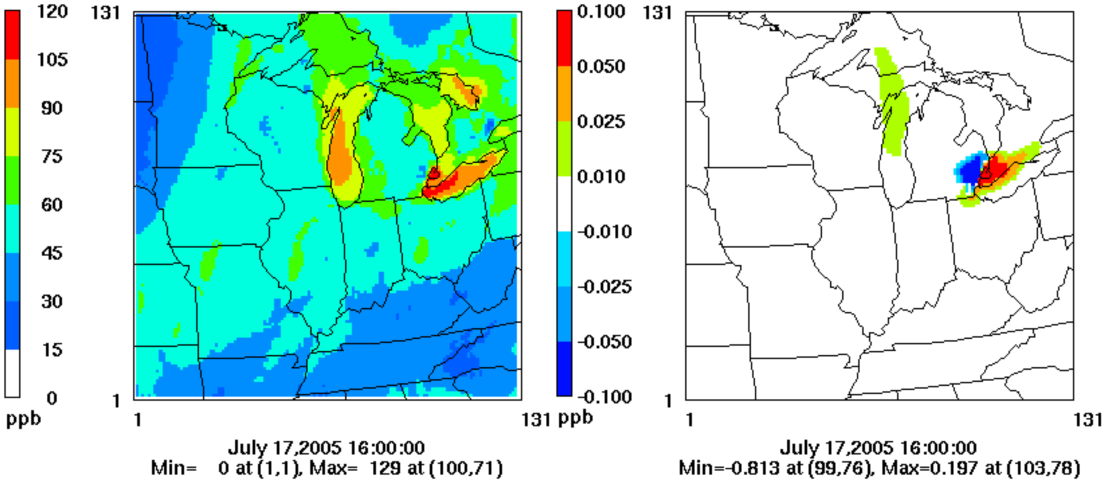

Figure 2-17. Impact of reformulated gasoline use in the SEMCOG network on surface ozone concentrations; 8-hour average (noon-7 PM EDT) ozone concentration due to conventional gasoline (left) and change due to reformulated gasoline (right) on July 17, 2005.

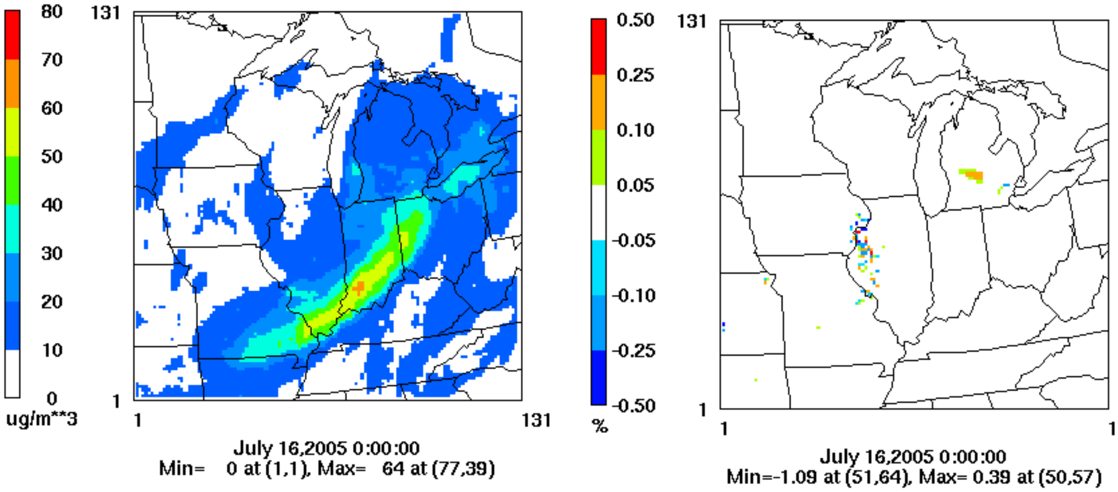

Figure 2-18. Impact of reformulated gasoline use in the SEMCOG network on surface PM concentrations; 24-hour average $PM_{2.5}$ concentration due to base fuel (left) and percent change due to reformulated gasoline (right) on July 16, 2005.

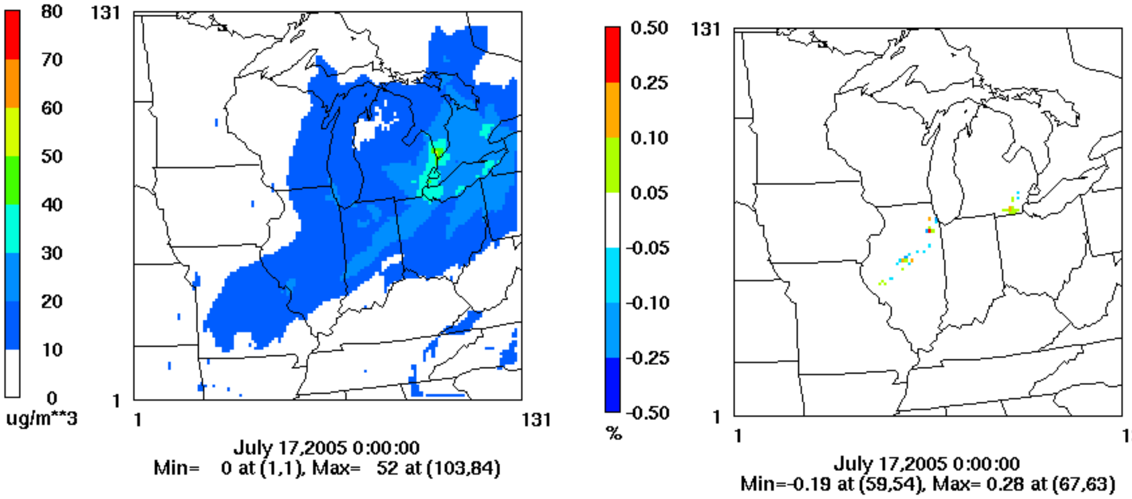

Figure 2-19. Impact of reformulated gasoline use in the SEMCOG network on surface PM concentrations; 24-hour average $PM_{2.5}$ concentration due to base fuel (left) and percent change due to reformulated gasoline (right) on July 17, 2005.

3. MODIFICATIONS TO THE CONCEPT-NONROAD MODULE

3.1. Incorporation of NONROAD2002 in CONCEPT

A flow chart representing the non-road mobile source module in CONCEPT is shown in Figure 3-1. As in the on-road module, a key feature of the non-road module is the interface between CONCEPT and EPA's NONROAD model (www.epa.gov/oms/ nonrdmdl.htm; Environ, 2002), which is used to estimate county level non-road emissions based on either default or user-defined input files. The temperature inputs to the NONROAD model are set to be 68-84 deg. F, with an average temperature of 75 deg. F. After the NONROAD model is run, results are imported back into the CONCEPT PostgreSQL database. Temporal allocation, speciation, and spatial allocation are then performed, followed by a temperature adjustment step based on input meteorology. The resulting data are output in gridded format.

We obtained an incomplete version of CONCEPT-Nonroad from LADCO in September 2009 (M. Janssen, personal communication, 2009) and with LADCO's assistance, we completed the implementation of NONROAD2002 in CONCEPT. This involved extensive analysis, debugging and testing of postgreSQL and Perl code and UNIX shell scripts. Though newer versions of NONROAD are available (the most recent being NONROAD2008), NONROAD2002 was selected based on CRC's recommendation; the implementation of NONROAD2008 into CONCEPT was deferred.

Changes were made to several of the modules shown in Figure 3-1 to enable the functioning of CONCEPT-Nonroad; the modules revised included 'initialization and setup', 'creation of NONROAD input files', 'speciation', 'spatial allocation' and 'temperature adjustment'. Some of the key updates are described briefly below.

The non-road driver script was updated to import meteorology and RPO cross-reference data. The format of the meteorology data was altered for consistency between the current version of CONCEPT and that available with the 4-RPO domain used for testing CONCEPT-Nonroad. The script to import the NONROAD2002 input data files was modified to include two additional tables. One of the tables (nonroad_fuelcon_to_nh3) was changed from globals to coarse schema. The nonroad_em and nonroad_fuelcon_to_nh3 postgreSQL tables were merged to create the nei_nonroad_em table. Organics were specified as VOC instead of HC in the run control file to be consistent with the use of VOC as a pollutant code in the nei_nonroad_em table. The NONROAD2002 parameters file was revised to be consistent with the specification of fields in the field_defs.dat file. The scripts nonroad_diurnaladj.sql, nonroad_mkcaludi_inp.sql and nonroad_tmpradj.sql were revised to enable them to work correctly. To circumvent the problem of excessive database commits resulting in CONCEPT run crashes, the continental US domain was split into five sets of states that were modeled separately.

PM_{10} (and not $PM_{2.5}$) is output by default from CONCEPT-Nonroad. NONROAD's reporting utility calculates $PM_{2.5}$ from PM10 by applying a factor as follows. For non-road engines, all PM emissions are assumed to be PM10, and 92% of the PM from gasoline and diesel fueled engines is assumed to be $PM_{2.5}$. For gaseous fueled engines (LPG/CNG), 100% of the PM emissions are assumed to be $PM_{2.5}$. This apportionment is performed in the reporting utility but not in the "core model" source code run on UNIX. To solve this problem, we set up a mapping between PM10 and $PM_{2.5}$ in the rpo_cp file (the chemical conversion profile file). We also added profile codes for non-road SCCs to the rpo_cr file (profile cross-reference table) and added the split factor for PM for those profile codes to the rpo_lp file (lumped profile speciation table).

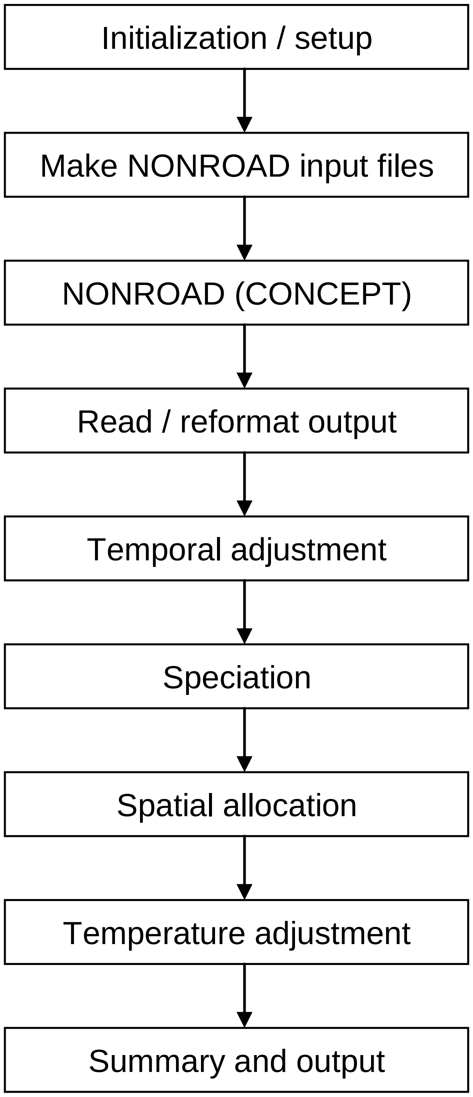

Figure 3-1. Flow chart representing the CONCEPT-Nonroad module.

3.2. Alternative fuel and technology module in CONCEPT-Nonroad

Figure 3-2 shows a flowchart representing the implementation of an alternative fuel and technology module in CONCEPT-Nonroad. There is a key difference between this implementation and that in CONCEPT-Mobile. MOBILE 6.2 outputs emission factors whereas NONROAD2002 outputs emissions (the reporting utility from NONROAD2005 onwards reports emission factors also). Thus, emission factors input to NONROAD are modified to account for the effect of switching to a renewable fuel. The factors are specified in the EMFAC (*.emf) files for exhaust HC, CO, NO_x and PM and crankcase and diurnal HC emissions read by NONROAD2002. The base fuel properties (fuel RVP, gasoline sulfur etc.) are provided in the NONROAD2002 input options file to calculate exhaust and evaporative emissions for the base case.

First the existing NONROAD2002 data files for technology types (tech.dat), deterioration factors (*.det files) and emission factors (*.emf files) are read. Then test data for new fuels and technologies are processed; these include the properties of the base and alternative fuel (such as conventional and reformulated gasoline), the observed emissions factors for these fuels, and test data on new technology types. User-provided data on SCC, horsepower and the fractions of the equipment population for different technology types in different years are used to revise the tech.dat file. New tech types may be defined for any SCC as long as the emission factors and deterioration rates are also provided for those new tech types. We re-normalize fractions of equipment population for the existing tech types so that the fractions for those types and the new tech type add up to 1. The *.det files (one for each of the pollutants CO, NO_x, HC and PM) contain deterioration factors that dictate the increase in emissions with equipment age. These files are revised using deterioration factor data for the new technology types. We revise fuel properties in the non-road parameters file for states/counties using the fuels of interest. These data are transferred to the NONROAD2002 options (*.opt) file by CONCEPT.

To revise the *.emf files, we first read user-provided test data that contains a fuel name/ID, SCC, model year, tech type, hp, pollutant name and emissions factor. We compare the SCC, tech type, hp combination against the records present in the revised tech.dat file and proceed if the combination is available. We assume that the new fuel is used only for the SCC and technology type, and hp indicated. All other technology types for this SCC and all other SCCs are assumed to use the default fuel in NONROAD2002.

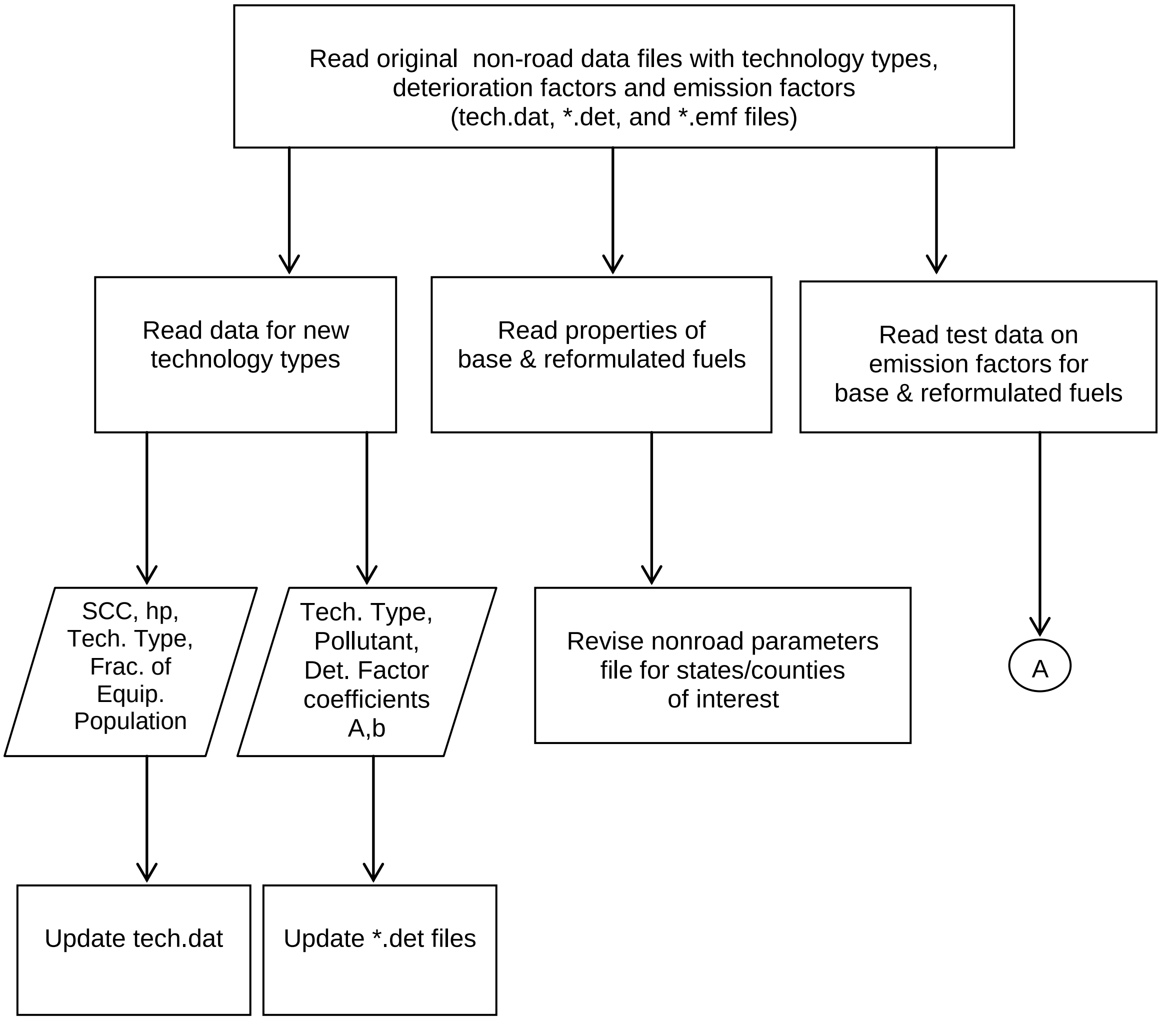

Figure 3-2. Flowchart representing the steps in implementing the alternative fuel and technology module in CONCEPT-Nonroad**.**

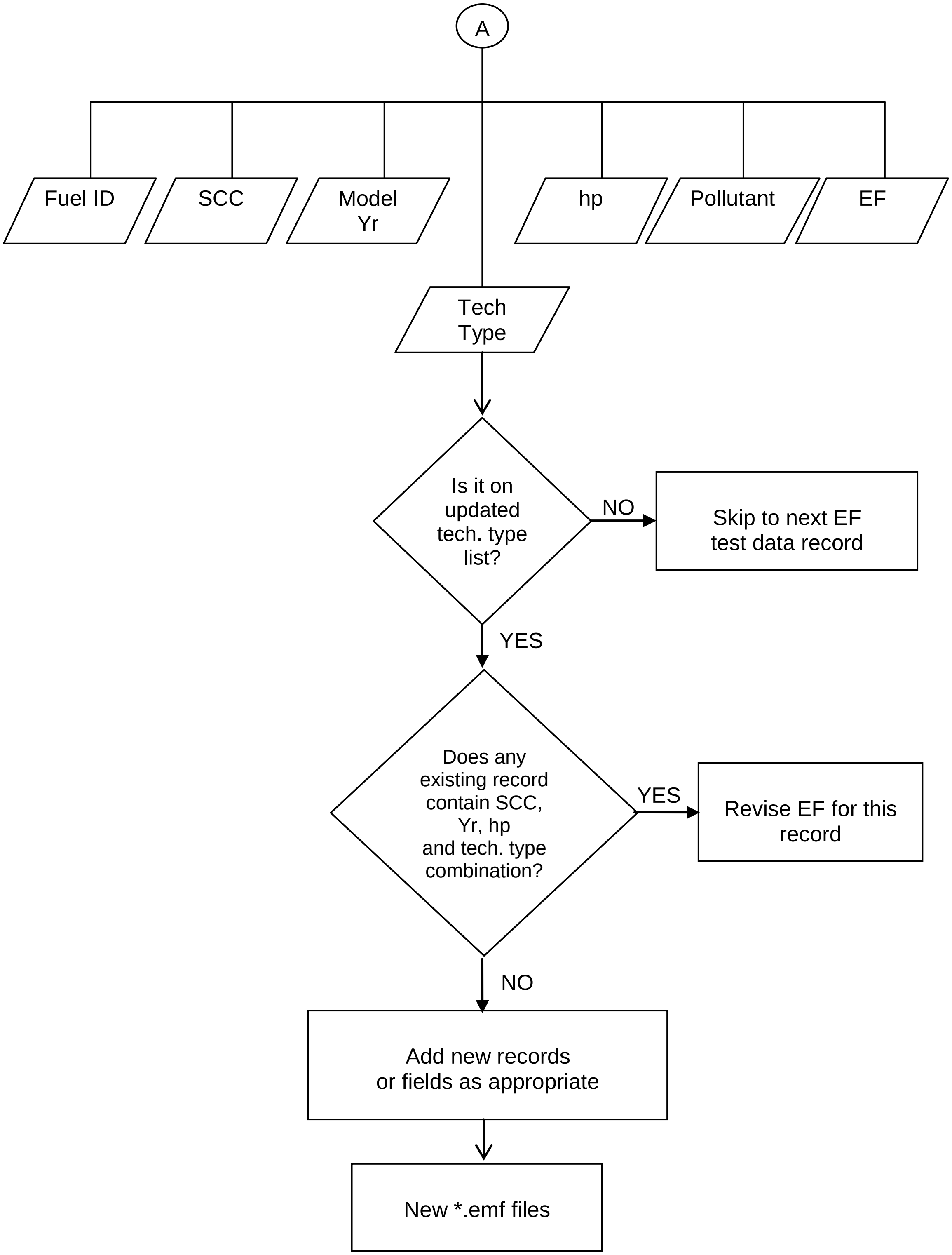

Figure 3-2 (continued). Flowchart representing the steps in implementing the alternative fuel and technology module in CONCEPT-Nonroad**.**

3.3. Test Application of the Alternative Fuel module in CONCEPT-Nonroad

Volckens et al. (2007) measured exhaust emissions from a series of small handheld, gasoline-powered 2-stroke engines used in string trimmers, leaf blowers, chainsaws etc. Emissions of CO, NO_x, HC, $PM_{2.5}$ and other pollutants were measured for new and used engines using conventional gasoline and gasoline with 10 volume percent ethanol blend (E10). Emission factors from this study were used to test the alternative fuel module in CONCEPT-Nonroad.

3.3.1. Impact of reformulated fuel use on non-road emissions

CONCEPT-Nonroad was run for all states in the continental US for July 15, 2005 and output emissions were converted to CAMx format. The CAMx emissions were extracted over a sub-domain over the central and eastern US at 36 km resolution (see outer domain in Figure 2-13). New emission factors (g/kW-hr) were provided for new string trimmers (SCC = 2260004025 and 2260004026) and chainsaws (SCC = 60004020 and 2260004021). Both types of equipment had a technology type of G2H4C2 (i.e., meeting Phase 2 standards and catalyst-equipped). Emission factors for these two equipment operated with conventional gasoline and E10 were applied in CONCEPT-Nonroad for Texas (only one state was chosen in this demonstration). All other states used the NONROAD2002 default fuel.

Figure 3-3 presents the daily ALD2 (acetaldehyde and higher molecular weight aldehydes) non-road emissions in the conventional gasoline scenario and the relative change in these emissions due to E10 use in trimmers and chainsaws in Texas on July 15, 2005. Similar plots are shown for CO, ethene (ETH), NO_x, olefins (OLE) and $PM_{2.5}$ in Figures 3-4 to 3-8. Non-road ALD2, ETH and OLE emissions decrease approximately by up to 0.4% in Texas with E10 use. Non-road CO emissions decrease by up to 0.25%. NO_x emissions show no noticeable change; emission factors for string trimmers increase and those for chainsaws decrease resulting in no net change (Volckens et al. 2007). The non-road $PM_{2.5}$ primary emissions decrease by up to 0.1% in isolated areas in Texas. Table 3-1 shows the statewide CONCEPT-Nonroad emissions in base and alternative fuel scenarios on July 15, 2005 in Texas. Total non-road emissions of CO and VOC in Texas decrease by approximately 0.2% due to E10 use in string trimmers and chainsaws in the state. Statewide total NO_x emissions do not exhibit a change. The net change in non-road PM emissions in Texas is also minimal.

3.3.2. Impact of reformulated fuel use on ambient ozone and PM

CAMx simulations were conducted for July 15, 2005 over the 36-km resolution domain. Other emissions files and other inputs were obtained from LADCO. Initial conditions were obtained from the last hour on July 14, 2005 of a prior annual CAMx simulation for 2005 available from LADCO.

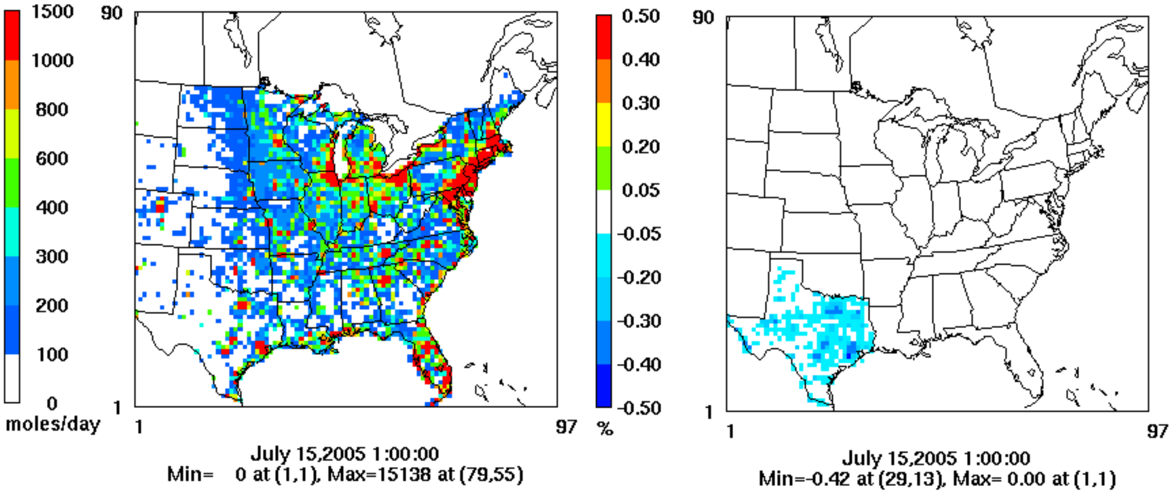

Figure 3-3. Daily non-road ALD2 emissions in conventional gasoline scenario (left) and percent change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

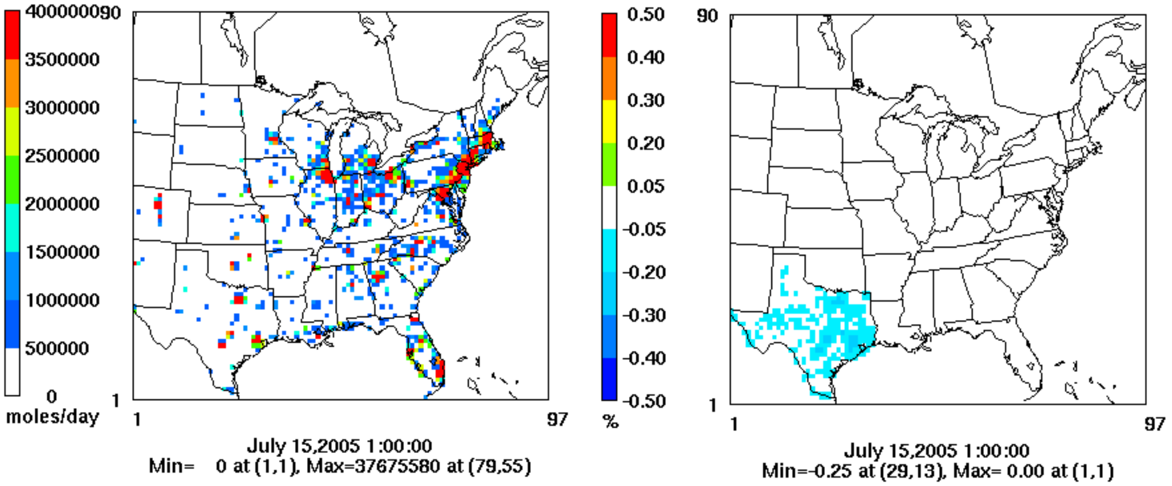

Figure 3-4. Daily non-road CO emissions in conventional gasoline scenario (left) and percent change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

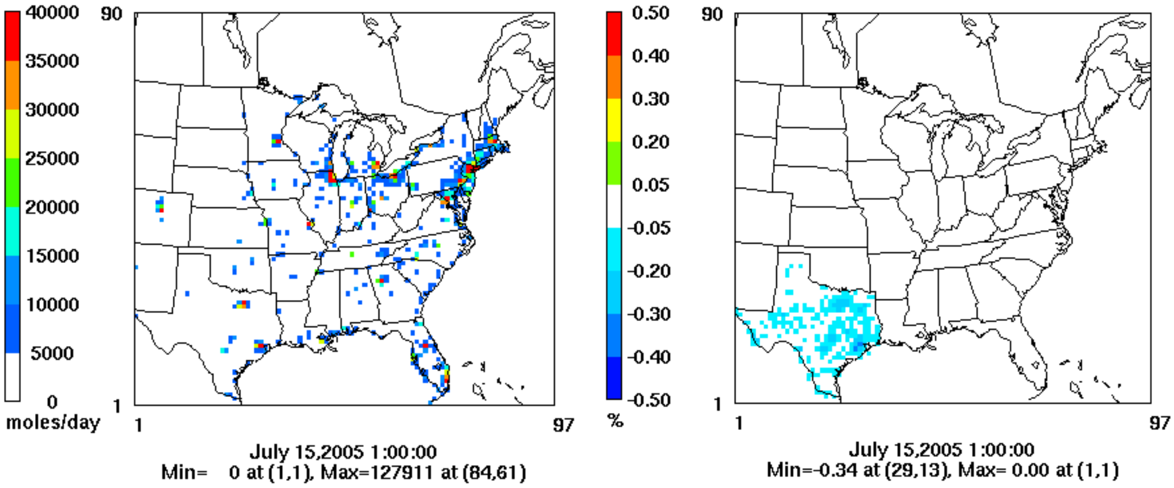

Figure 3-5. Daily non-road ETH emissions in conventional gasoline scenario (left) and percent change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

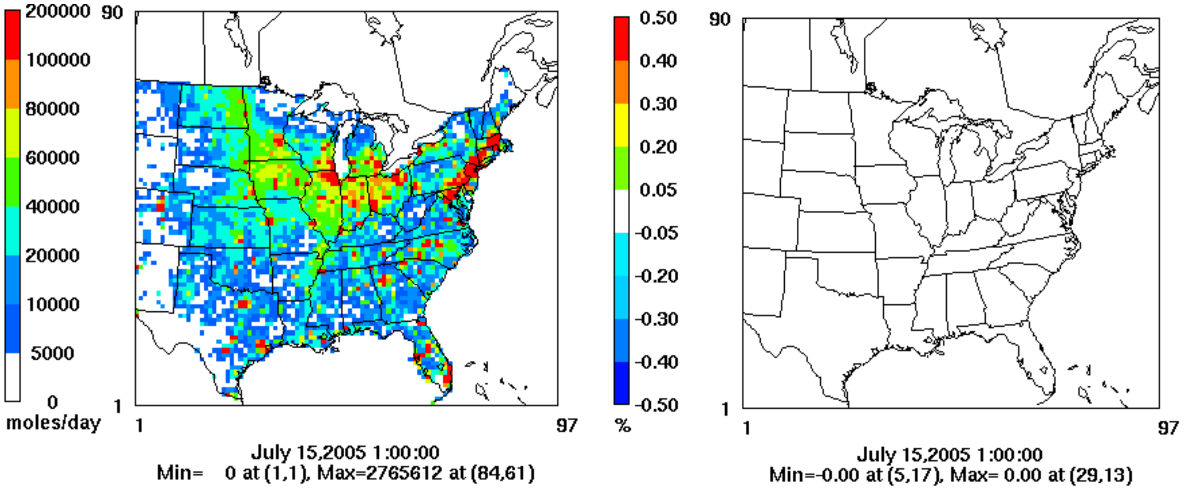

Figure 3-6. Daily non-road NO_x emissions in conventional gasoline scenario (left) and percent change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

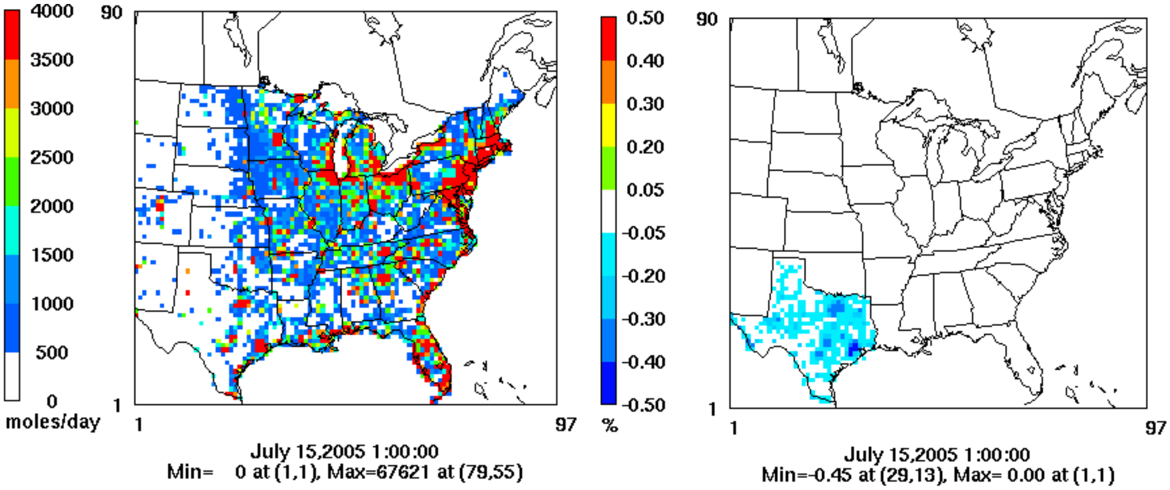

Figure 3-7. Daily non-road OLE emissions in conventional gasoline scenario (left) and percent change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

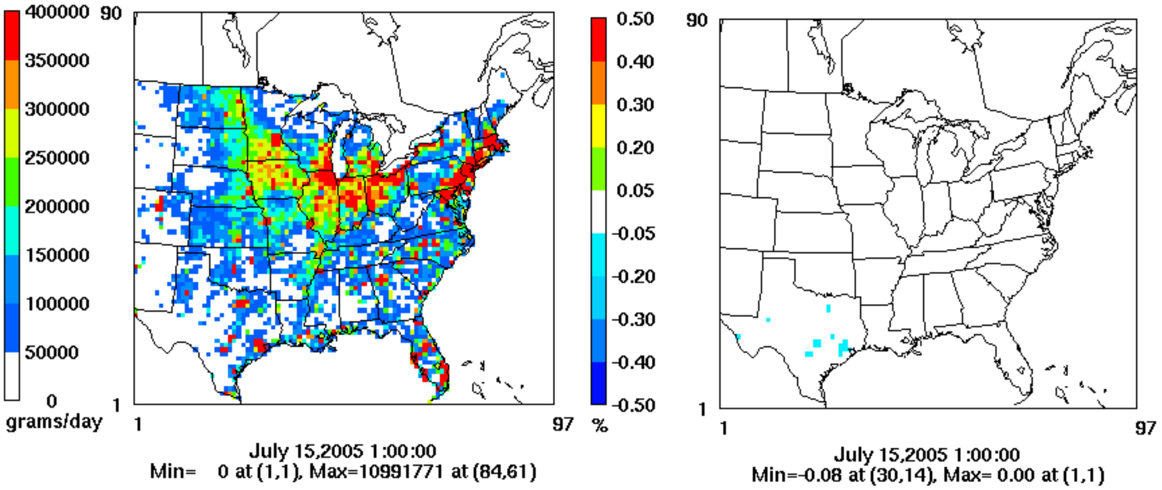

Figure 3-8. Daily non-road $PM_{2.5}$ emissions in conventional gasoline scenario (left) and percent change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

Table 3-1. Emissions in base and alternative fuel scenarios on July 15, 2005 from the CONCEPT-Nonroad module.

Species	**Texas non-road emissions (base fuel scenario) (tons/day)**	**Texas non-road emissions (alternative fuel scenario) (tons/day)**	**Change in Texas non-road emissions between base and alternative fuel scenarios (%)**
CO	4549	4542	-0.17%
NO_x	496	496	0.00%
VOC	353	352	-0.24%
PM	52	52	-0.02%

CAMx simulations were conducted over the 36-km resolution domain using the CONCEPT-Nonroad emissions for conventional gasoline and E10 for July 15, 2005. New emission factors were used only for string trimmers and chainsaws in Texas; others used the NONROAD2002 default. Other emissions data and other inputs were obtained from LADCO and were held constant between the base and alternative fuel scenarios. Figure 3-9 shows the peak hourly surface ozone concentrations in the base fuel scenario on July 15, 2005 and the change in hourly surface ozone at the hour of maximum change due to use of E10 in Texas. Similar plots are shown for the surface 8-hr ozone (from noon to 7 pm EDT) and 24-hr average $PM_{2.5}$ concentrations in Figures 3-10 and 3-11. There is negligible change in hourly and 8-hour ozone. Minor $PM_{2.5}$ impacts (up to 2-3% changes in 24-hour surface concentrations) are seen in isolated areas in Texas and other states due to transport. It should be noted that the test-case presented here is only a "proof of performance" demonstration and these results should be interpreted with caution.

Prior to running CONCEPT, the non-road inputs need to be modified. The time required to set up one CONCEPT run is approximately 15-30 minutes if the emission factors are available. CONCEPT-Nonroad is run for 10 states at a time instead of the whole continental U.S. to avoid memory problems caused by excessive data transfer with the postgreSQL database. The computational time for one CONCEPT-Nonroad run is approximately 5.5 hours for one day (for each set of 10 states) which is approximately equivalent to 27 hours for one day in the continental US domain at 36 km resolution. This is using an AMD Opteron 290 2.8 GHz processor. Thus CONCEPT Non-road is also very CPU intensive like the CONCEPT on-road module. The time specified includes the last step of the CONCEPT processing, i.e., creation of the CAMx non-road emissions file. After the CONCEPT run, the CAMx non-road emissions file created by CONCEPT has to be merged with other emissions to create the final CAMx-ready low-level emissions file. This process is quick (<10 minutes) if the other emission files are available.

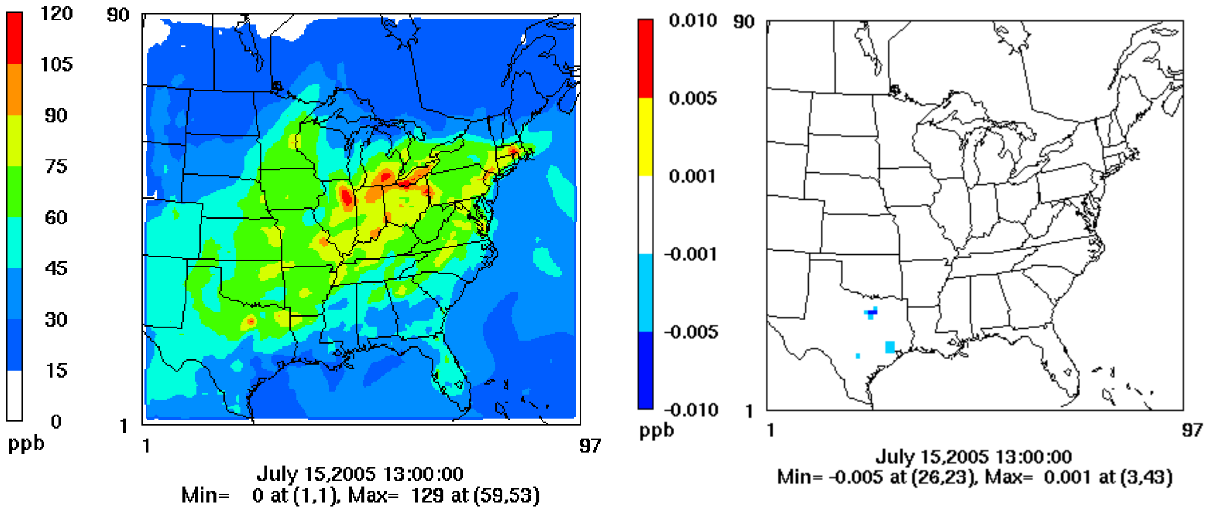

Figure 3-9. Impact of E10 use in Texas on surface ozone concentrations; peak hourly ozone concentration due to conventional gasoline (left) and change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

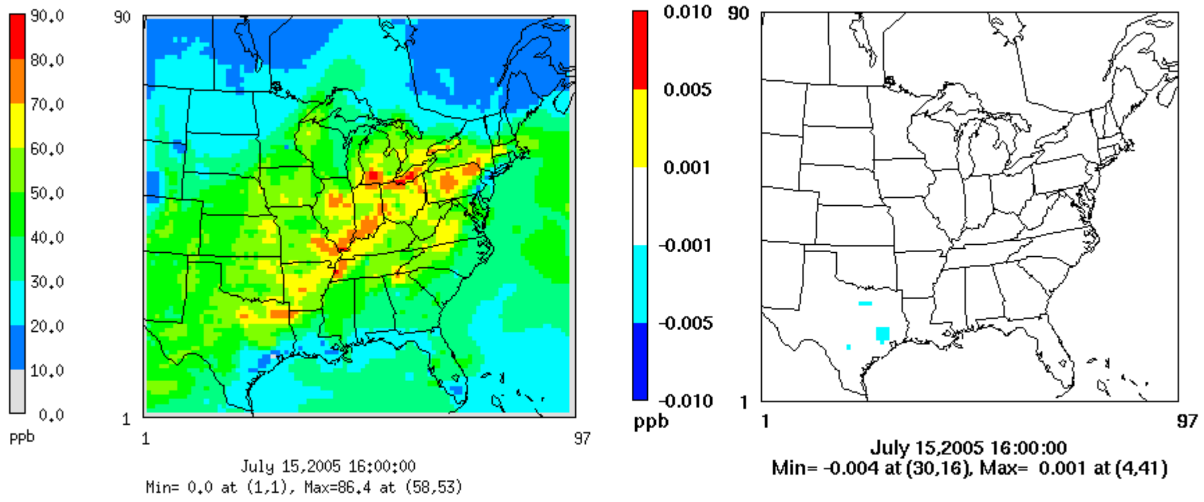

Figure 3-10. Impact of E10 use in Texas on surface ozone concentrations; 8-hour average (noon-7 PM EDT) ozone concentration due to conventional gasoline (left) and change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

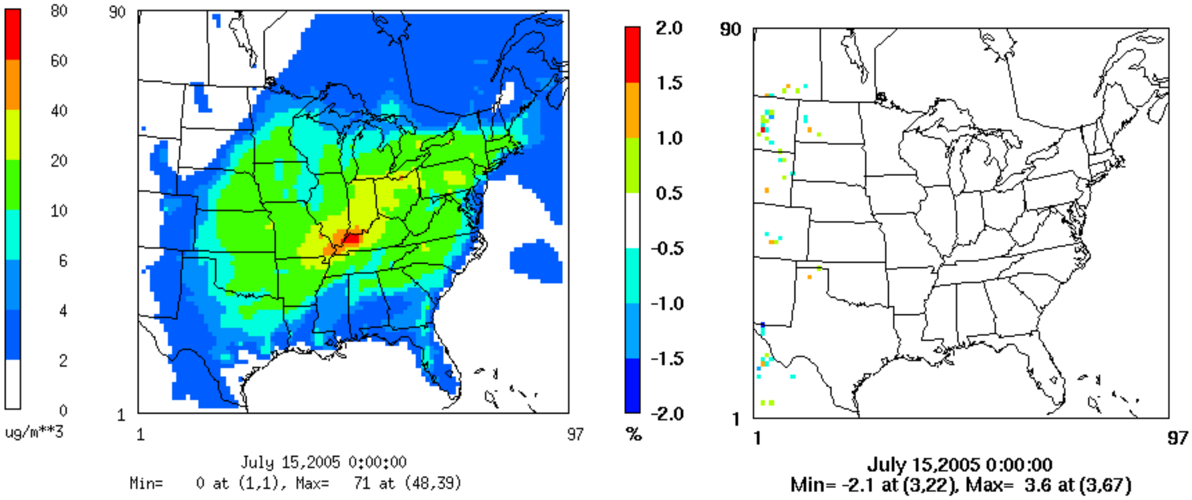

Figure 3-11. Impact of E10 use in Texas on surface PM concentrations; 24-hour average $PM_{2.5}$ concentration due to conventional gasoline (left) and change (right) due to E10 use in small two-stroke non-road equipment (trimmers and chainsaws) in Texas on July 15, 2005.

4. SUMMARY

The focus of this study was to provide the proof of concept of a modeling suite comprising CONCEPT and CAMx for the future study of the relationship between reformulated fuel use and ambient air quality. Several tasks were performed to achieve this goal.

The on-road mobile source module in CONCEPT was updated to incorporate flexibility for user-provided data on emissions due to alternative fuel and technology use. CONCEPT was also modified to use the standard EPA version of MOBILE6.2 and selected post-processing routines were altered to decrease computational time requirements. Unlike the version of MOBILE implemented in CONCEPT-Mobile, the standard EPA version provides disaggregated emission factors for 25 model years and 28 vehicle types which enable us to more easily model the effect of new fuels and technologies. Alternative emission factors can be provided to CONCEPT from any source of information (e.g., vehicle test data). Here, the California Predictive Model was used as an example to provide emission factors for base fuel (conventional gasoline) and alternative fuel (Federal reformulated gasoline) in the SEMCOG network area. These emissions were used to conduct CAMx simulations over a domain at 12 km resolution in the Upper Midwest. Other CAMx inputs were identical between the base and alternative fuel scenarios. Small impacts (<1 ppb) on surface ozone were simulated in Michigan and neighboring states due to the RFG use. $PM_{2.5}$ impacts were small as well but farther away. These results do not account for fuel trends such as the increasing use of ethanol in gasoline and hence are over-estimates of the actual impact of reformulated use on emissions and air quality. The results are not intended to be a comprehensive representation of alternative fuel impacts, rather a demonstration of the utility of the CONCEPT/CAMx model suite.

The implementation of NONROAD2002 in the version of CONCEPT provided by LADCO was completed by AER with LADCO's assistance. A method to account for alternative fuel and technology was also developed and tested in the CONCEPT-Nonroad module. Emission factor measurements for small two-stroke gasoline-powered handhelds (trimmers and chainsaws) published in the literature for conventional gasoline and E10 were used in CONCEPT-Nonroad modeling. The impact of the use of E10 in trimmers and chainsaws in Texas on ozone and $PM_{2.5}$ concentrations was tested with CAMx simulations over a domain at 36 km resolution over the central and eastern United States. Changes in non-road emissions due to the limited E10 use examined here are very small and result in negligible changes in surface ozone concentrations and small changes in surface $PM_{2.5}$ concentrations outside Texas. The emissions modeling and simulation discussed here are conducted over a short time period (one-day); they serve only as examples of the CONCEPT/ CAMX suite and should not be generalized.

5. ACKNOWLEDGEMENTS

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