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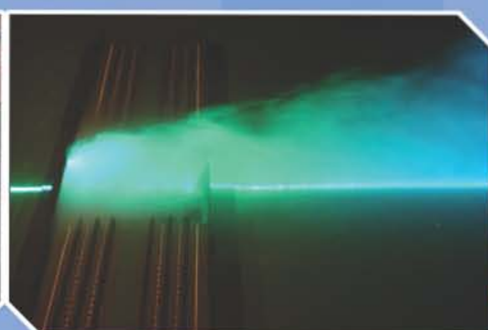


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Emission and Air Quality Modeling Tools for Near-Roadway Applications

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Table of Contents

List of Tables

1. INTRODUCTION

In the United States, more than 35 million people live within 100 m of a major roadway. A growing body of literature suggests that adverse health effects are associated with populations living near major roadways (e.g., Harrison et al., 1999; Brauer et al., 2002; Hoek et al., 2002; Finkelstein et al., 2004). According to U.S. Environmental Protection Agency (EPA) estimates from 2006, highway sources contribute 22% of volatile organic compounds (VOCs), 36% of nitrogen oxides (NO_x), and 54% of carbon monoxide (CO) of all anthropogenic emissions. Despite cleaner fuels and improved onboard emission control technology, the growth of vehicular miles traveled and traffic congestion in urban areas may further exacerbate the impact of roadway emissions on air quality and human health.

Air quality modeling of emissions from roadways usually is applied either for regulatory purposes or for supporting health studies. From a regulatory perspective, State and local authorities are required to consider the impact of roadway emissions on air quality as part of the State Implementation Planning (SIP) process and to demonstrate that transportation-related projects do not cause or worsen air quality (formally defined as a “transportation conformity” analysis). Although epidemiological studies, as well as toxicology studies, show associations between exposure to traffic near major roadways and elevated risks of adverse health effects, such as asthma, impaired cardiovascular function, and diminished life expectancy, other epidemiological studies highlight the need to resolve spatial gradients near roadways, because, if concentration profiles are spatially variable, the analysis of particulate matter (PM) air pollution and health data could be compromised by exposure misclassification errors (U.S. EPA, 2004).

The typical set of tools for estimating near-road air quality consists of estimates or measures of traffic activity, calculation of roadway emissions, and analysis of ambient air concentrations with a numerical air quality model using estimated emissions. To our knowledge, a comprehensive review of roadway emission and near-roadway air quality models does not exist, and sources of information on air quality and emission modeling of roadways are diverse and scattered. For example, Jungers et al. (2006) provide a survey of dispersion models for use in conformity analysis in California. In this document, we review emission and air quality modeling techniques for estimating airborne emissions from roadways. Each model was reviewed for the following attributes: (1) model name, (2) developer name and affiliation, (3) scope of application, (4) URL addresses (if available), (5) summary of model input requirements, (6) summary of model technical formulation, (7) discussion of model strengths and limitations, and (8) references of supporting model documentation.

Nine emission models (Section 2) and 21 air quality models (Section 3) are identified and discussed in this document. The models are described, along with a description of their strengths and weaknesses. In Section 4, the strengths and weaknesses of existing operational modeling tools are summarized, and areas of improvement to assist in assessments of air pollutant impacts near roadways are recommended. The intent of this review is to provide a convenient compendium of existing operational modeling techniques and to provide guidance for researchers interested in improving the accuracy of air quality modeling for near-road applications.

2. EMISSION MODELS

One of the first steps in performing a near-roadway air quality assessment is to estimate air pollutant emissions from the roadway environment. Currently, modal and nonmodal models provide emission estimates. Modal models generate emission factors to account for differences in vehicle operation (i.e., idle, steady-state cruise, acceleration/deceleration), whereas nonmodal models generate emission factors for average vehicle speeds over different driving cycles. The emission factors are combined with vehicle activity data, usually in the form of distance traveled, to estimate emissions. Then, the resulting emission inventory or emission factors are used as inputs to air quality models, depending on the input requirements of the air quality model. This review of nine emission models is separated into current operational models and research-grade models. The emissions models, their developers and reference web sites are listed in Table 1.

Table 1. Summary of Emission Models

Model Name	Developer	URL
Current Operational Models		
Consolidated Community Emissions Processing Tool (CONCEPT)	Lake Michigan Air Director's Consortium/ Midwest Regional Planning Organization	http://www.conceptmodel.org/
Emission Factors (EMFAC)	California Air Resources Board	http://www.arb.ca.gov/msei/onroad/latest_version.htm
MOBILE6.2	U.S. EPA	http://www.epa.gov/otaq/m6.htm
Motor Vehicles Emissions Simulator (MOVES)	U.S. EPA	http://www.epa.gov/otaq/ngm.htm
Research-Grade and European Models		
Comprehensive Modal Emissions Model (CMEM)	University of California, Riverside	http://pah.cert.ucr.edu/cmem/
COPERT	European Environment Agency	http://lat.eng.auth.gr/copert/
Microscale Emission Factor (MicroFac)	Dr. R. Singh (University of Waterloo)/U.S. EPA	http://dx.doi.org/10.1016/j.atmosenv.2006.04.012
Mobile Emissions Assessment System for Urban and Regional Evaluation (MEASURE)	Georgia Institute of Technology/U.S. EPA	http://gtresearchnews.gatech.edu/reshor/rh-spr99/tr-emis.html
Transportation Analysis Simulation System (TRANSIMS)	Los Alamos National Laboratory	http://tmip.fhwa.dot.gov/transims/

2.1. Current Operational Emission Models

Currently, four models are used widely in the United States for estimating mobile source emissions for air quality modeling applications, which may or may not be applicable to near-road situations.

2.1.1. Consolidated Community Emissions Processing Tool (CONCEPT)

CONCEPT is a suite of independent models that use common supporting routines and formats. It is an open-source model that combines attributes of current emissions modeling systems. Most, if not all of the software, is in the public domain, and users are encouraged to customize and share it. CONCEPT has the following models that are in various stages of development: (1) area sources, (2) point sources, (3) onroad motor vehicles, (4) nonroad motor vehicles, (5) biogenic sources, and (6) process-based livestock ammonia model.

The CONCEPT onroad motor vehicle model combines vehicle activity data (volumes, speeds, and trip counts) with motor vehicle emission factors derived from a modified version of EPA's MOBILE6 model to generate hourly, model-ready emissions estimates. Estimates of emissions during refueling are not modeled by CONCEPT.

CONCEPT's onroad motor vehicle model is designed to obtain activity data from the Transportation Demand Model Transformation Tool (T3). Users must provide the following information: input data describing the characteristics of the motor vehicle fleet, spatial allocation of roadway characteristics (roadway design/type of roadway, number of lanes/capacity, speed limit, etc.), chemical speciation mechanism (i.e., CBIV, SAPRC), MOBILE6 cross-reference data and execution parameters, modeling episode, modeling grid definitions, and the required air quality model output format (CMAQ or CAMx). Other input data inputs for CONCEPT include vehicle miles traveled, number of trips, volumes, network capacity, speeds, network definitions, speed adjustments, and meteorological data.

The onroad motor vehicle source model combines MOBILE6 emission factors with link-based or county-level vehicle activity data. CONCEPT uses T3 to generate link-based vehicle activity data. The model generates a MOBILE6 run for a number of variables: representative county, minimum/maximum temperature, calendar year, season, roadway type, and speed bin.

Runs are made within CONCEPT for freeway and arterial roadways. In addition, speeds are "hard-coded" in MOBILE6 for freeway ramps and local roads. Emissions are allocated temporally by applying profiles by State, county, roadway type, year, month, and day of week. Temporal adjustments also are applied to vehicle miles traveled, volume, capacity, and trip counts. This is especially critical when looking at heavy-duty diesel vehicles because weekend/weekday variations, including hourly variation, can have a significant impact on emissions.

The T3 model disaggregates traffic volumes for multihour periods into hourly volumes, and the data are based on analyses of calendar year 2002 automated traffic recorder data. The hourly total volume profiles are developed to correspond to the facility class, month, and day of week provided by the Department of Transportation's Highway Performance Monitoring System. The automated traffic recorder data appears to be available for only a handful of States, and an Internet query indicates that the data are easily accessible only for Minnesota. A presentation prepared by Environ and the Lake Michigan Air Directors Consortium (LADCO) indicates that T3 analyses have been performed only for Illinois, Michigan, Minnesota, and Wisconsin.

The current version of CONCEPT provides emissions-related information for hydrocarbons (HC), CO, and NO_x. Because CONCEPT makes use of MOBILE6, it is being used to provide emissions estimates for hazardous air pollutants (HAPs) and PM, as well as sulfur dioxide (SO_2). EPA currently is customizing CONCEPT to provide hazardous air pollutant emissions modeling capabilities.

One of the apparent strengths of CONCEPT is that it relies on open-source models. In addition, the model is designed to be transparent and to allow multiple levels of quality assurance (QA) analysis. The model uses MOBILE6 to generate emissions factors. In general, CONCEPT's strength appears to be its application to the regional/urban scale.

A potential weakness of the CONCEPT model is that it has not been finalized. In addition, many of the components of CONCEPT have not been beta tested. However, discussions with the model developers indicate that the mobile source module is robust; it relies on the MOBILE6 platform, which has been evaluated and applied extensively. The most significant problem with CONCEPT is that it is relatively early in its development, and its development has focused on QA and transparency in lieu of development on processing efficiency and model speed.

Another potential weakness is that CONCEPT generally uses Bureau of Public Records speed curves, which may not be the most accurate approach to estimating vehicle speed. This methodology assigns the same speed to all vehicles for a roadway link independent of whether the vehicles are light or heavy duty.

The CONCEPT model does not appear to be adapted for microscale applications, such as is the focus of EPA's near-roadway research initiative. Output is oriented toward the county level, and the current version appears to have been applied only to the Midwest (LADCO), where the proper traffic data has been made available. Although emissions factors are developed using MOBILE6, they are combined with link-based or county-level activity data. The motor vehicle model is also perhaps overly input demanding considering that some applications require only a 1-km stretch of urban interstate. This stretch of road does not have any significant increases or decreases in height, and it can be assumed that most vehicles are traveling at fairly consistent speeds; therefore, it is faster, easier, and simpler to run MOBILE6 and apply vehicle-miles-traveled (VMT) estimates to the emissions factors to develop an emissions inventory.

CONCEPT enables input of vehicle activity data using any set of vehicle types. However, the MOBILE6 emission factors are generated in terms of the eight MOBILE5 vehicle classes. Therefore, all incoming activity data must be allocated to these eight classes, which require a file that cross-references the activity data to the MOBILE5 classes.

Unlike other models, the CONCEPT system requires a number of software packages to be downloaded, installed, and configured prior to the installation of the CONCEPT model itself. Such packages include PostgreSQL, PostGIS, PROJ.4, GEOS, and ActivePerl. The user's guide also recommends the installation of a FORTRAN compiler and IO/API with National Center for Atmospheric Research netCDF libraries.

2.1.2. EMFAC2002/2007

EMFAC2007 calculates emissions inventories for pollutants from onroad motor vehicles operating in California. EMFAC is a FORTRAN computer model capable of estimating both current year and back-cast and forecasted inventories for calendar years 1970 to 2040. EMFAC estimates the emission rates of 1965 and newer vehicles powered by gasoline and diesel fuels. Emissions estimates are made for over 100 different technology groups and are reported for three distinct vehicle classes segregated by usage and weight.

EMFAC calculates the emission rates of total organic gas, reactive organic compounds, HC, CO, NO_x, PM, PM_{10}, $PM_{2.5}$, lead, SO_2, methane (CH_4), and carbon dioxide (CO_2) for 45 model years for each vehicle class within each calendar year; for 24 hourly periods; for each month of the year; and for each county, air basin, and air management district in California. EMFAC can report the grams-per-mile emission rates of a single technology group or the tons-per-day inventory for the entire 28-million-vehicle California fleet. With the exception of lead, EMFAC does not calculate the emission rates for hazardous air pollutants. A separate "speciation" step therefore is required, using factors provided by the Air Resources Board (www.dot.ca.gov/hq/env/air/pages/msat.htm).

EMFAC2007, like previous versions of the EMFAC modeling system, was designed primarily as an emissions inventory tool for air quality planning. EMFAC can be run over a number of calendar years to establish emissions reductions trends and determine reaction of the inventory to increases or decreases in population and VMT. Therefore, the model is a useful tool for trend analyses, an essential tool in assessing "progress versus plan" for air quality planning in California, and a vital tool for determining the regulatory benefits and cost effectiveness of specific emission reduction strategies or the overall effects of growth and control.

The EMFAC modeling system is tailored specifically to California in that geographical inputs are specific to this State, and the model covers California-specific light-duty vehicle standards, as well as inspection and maintenance programs. Several scenario types can be modeled: (1) BURDEN (to provide an area planning inventory in tons per day), (2) EMFAC (to provide area fleet average emissions in grams per hour), and (3) CALIMFAC (to provide detailed vehicle emissions data in grams per mile). Model inputs include geographical area, calendar year, month/season, and beginning and final model years of vehicles being modeled. EMFAC2007 has a scenario-generating tool that allows input of various model options and scenarios, such as inspection and maintenance assumptions, various correction factors, outputs specific to Federal Test Protocol bags, vehicle population data and odometer accrual values, number of trips per day and the accrued VMT, Reid vapor pressure of the fuel, ambient temperature and relative humidity profiles, speed fractions, and idle times.

EMFAC is a FORTRAN model that is constructed in a “bottom-up” fashion. Therefore, the model is constructed from test data with no preconceived assumption regarding the end result. Special test programs and research projects have been conducted to isolate single variables such as speed and temperature to determine their relative effects on emissions. Multivariate tests also have been run to determine whether interactions exist among variables. These data ultimately are reduced to mathematical equations called “correction factors,” which are applied to a “basic emission rate” or a base assumption of a vehicle’s emission characteristics.

Designed primarily as a planning tool, the EMFAC modeling system is maintained and updated by the California Air Resources Board (CARB) as statewide and regional SIPs are updated. Because EMFAC was designed as a California-specific planning tool, the model focuses on vehicles operating in California at a statewide and regional level. The model is not designed to estimate subregional inventories on a link- or grid-specific basis and is not designed for conducting assessments on vehicle fleets that do not operate in California.

EMFAC model outputs commonly are used for project-level air quality assessments. For example, CARB has conducted health risk assessments of emissions generated at ports and railyards throughout California (http://www.arb.ca.gov/ports/ports.htm; http://www.arb.ca.gov/railyard/railyard.htm). In these studies, EMFAC emission rates were used in conjunction with vehicle volumes and speeds on a roadway network to estimate emissions. EMFAC emission rates also are used routinely to support air quality assessments through the California Environmental Quality Act. With new State-level requirements to assess greenhouse gas emissions associated with the transportation and goods movement sectors, as well as new regulations designed to reduce criteria pollutant emissions from diesel vehicles and new initiatives to assess subregional and local-scale health risk, modeling requirements on the EMFAC modeling system are expanding. In recognition of these expanded requirements, CARB is developing a toolkit of next generation emissions models designed to assess greenhouse gas, criteria, and toxic air pollutants at statewide, regional, and local scales that integrate VMT estimates from EMFAC vehicle modeling and from statewide/regional travel demand modeling and that integrate statewide fuel usage estimates with vehicle activity estimates.

A user’s guide and training materials are available from CARB’s Web site.

2.1.3. MOBILE6.2

MOBILE6.2 is an emission factor model designed by EPA to estimate emission rates for the highway motor vehicle fleet under a wide range of conditions. MOBILE6.2 is the latest in a series of MOBILE models dating to 1978. One of the primary uses of the MOBILE model is to develop emission inventories for SIPs and for conformity determinations. It has been used widely for mobile source emission inventory development efforts at many spatial resolutions. MOBILE6.2 has a variety of output formats, but, specifically, it provides emissions factors by vehicle types. These emissions factors, when combined with activity data (VMT), provide emissions estimates that can be used in the development of emissions inventories or as inputs to air quality models. MOBILE6.2 enables users to calculate and report emissions factors by category for some pollutants. For example, evaporative HC emissions from gasoline-fueled vehicles include diurnal emissions, hot soak emissions, running losses, resting losses, and refueling emissions. Similarly, MOBILE6.2 can report emissions by roadway type, time of day, vehicle category, and other characteristics that allow for very detailed modeling of specific local situations. MOBILE6.2 is not, however, a modal emissions model. MOBILE6.2 is not designed to produce second-by-second emission rates or emission rates for individual vehicles in the traffic stream that may have variable driving patterns. Also, it is not applicable in situations where automobiles are driven in transition between two segments of roadway with different average speeds.

MOBILE6.2 includes default values for a wide range of conditions that affect emissions. Worth noting is a correction for aggressive driving behavior. The defaults are designed to represent "national average" input data values. Users who desire a more precise estimate of local emissions can substitute information that more specifically reflects local conditions. Use of local input data is particularly common when the customization and development of emissions inventories or other modeling efforts are constructed from separate estimates of roadways, geographic areas, or times of day in which fleet or traffic conditions vary considerably. MOBILE6.2 is used to develop emission inventories on various geographic scales.

MOBILE6.2 provides estimates of current and future emissions from as many as 28 vehicle classifications of highway motor vehicles. The model calculates average in-use fleet emission factors and can be programmed (via the input file) for the following roadway types: freeway, arterial, local, and freeway ramp.

MOBILE6.2 also calculates emissions for 10 emissions scenarios. Table 2 provides the emission type classifications and the pollutants for which emission factors are calculated.

MOBILE6.2 is designed to be used in conjunction with data created by traffic planners and, as such, is compatible with planning tools. It also uses facility-specific driving cycles to better differentiate speed effects on highways and arterials. Input files for the model can be developed that have high levels of customization, or a user can choose to use MOBILE6.2 default values. Specific MOBILE6.2 input parameters include the following: calendar year, month, weekend/weekday flag, hourly temperature, altitude, humidity, and solar input. The model also requires vehicle fleet information (registration distribution by vehicle class, annual mileage accumulation by vehicle class, diesel sales fractions by vehicle class and model year, natural gas vehicle fractions, average speed distribution by hour and roadway, distribution of vehicle miles traveled by roadway type and by vehicle class, and average trip length distribution) and fuel inputs (fuel characteristics, emissions factors for PM and HAPs, and particle size cutoff).

MOBILE6.2 is FORTRAN based and uses statistical relationships based on thousands of emission tests performed on both new and in-use vehicles. MOBILE6.2 is available for downloading from EPA's Web site. There is also ample documentation, along with a detailed user's guide and sample run data. EPA has produced 48 reports explaining the technical formulation of MOBILE6.2, which are available at www.epa.gov/otaq/models/mobile6/m6tech.htm. Unlike some of the other emission models, obtaining a copy of the program is straightforward.

MOBILE6.2 can generate emission factors for 28 types of highway vehicle classifications for criteria and HAPs: gaseous HCs, CO, NO_x, CO_2, sulfate, organic carbon, elemental carbon, total carbon portion of gasoline exhaust particulate, lead, SO_2, ammonia, brake and tire wear particulate, benzene, methyl tertiary butyl ether, 1,3-butadiene, formaldehyde, acetaldehyde, and acrolein. In addition, PM emission factors are based on algorithms from EPA's PM model, PART5. There are several

Table 2. Mobile Emission Type Classifications

Number	Abbreviation	Description	Pollutants[a]	Vehicle Classes
1	Running	Exhaust running emissions	All except tire and brake wear particulate	All
2	Start	Exhaust engine start emissions (trip start)	HC, CO, NO_x, toxics	Light-duty vehicles and motorcycles
3	Hot Soak	Evaporative hot soak emissions (trip end)	HC, BZ, MTBE	Gasoline, including motorcycles
4	Diurnal	Evaporative diurnal emissions (heat rise)	HC, BZ, MTBE	Gasoline, including motorcycles
5	Resting	Evaporative resting loss emissions (leaks and seepage)	HC BZ, MTBE	Gasoline, including motorcycles
6	Run Loss	Evaporative running loss emissions	HC, BZ, MTBE	Gasoline, including motorcycles
7	Crankcase	Evaporative crankcase emissions (blow-by)	HC	Gasoline, including motorcycles
8	Refueling	Evaporative refueling emissions (fuel displacement and spillage)	HC, BZ, MTBE	Gasoline, including motorcycles
9	Brake Wear	Particulate matter from brake component wear	Brake wear particulate	All
10	Tire Wear	Particulate matter from tire wear	Tire wear particulate	All

[a]The Additional HAPS command in MOBILE6.2 enables users to specify any compound either as a single emission rate or as a ratio to volatile organic compounds (VOCs) or particulate matter. For example, quinine emissions, not explicitly modeled in MOBILE6.2, can be modeled if the user has appropriate speciation data. In addition to the hazardous air pollutants specifically modeled by MOBILE6.2 (and included in this table), other VOCs can be modeled with the Additional HAPS command. This applies to all evaporate processes.
Pollutants: BZ = benzene, CO = carbon monoxide, HC = hydrocarbons, MTBE = methyl tertiary butyl ether, NO_x = nitrogen oxides

deficiencies in estimating PM emission factors in MOBILE6.2, primarily the result of carrying over the algorithms from PART5, the previous PM emission factor model. Delucchi (2000) found that PART5 "underestimates emissions from real on-road vehicles, primarily because PART5 seems to be based on low-mileage, properly functioning vehicles, and takes little, if any account of super-emitters." It also is thought that the database used to develop emission factors does not "include a representative number of old, malfunctioning, poorly tuned, or inherently high emitting vehicles." He also notes that real PM emissions may be higher by a factor of two than those estimated by PART5. PM emission rates are not sensitive to vehicle speed, road type, and temperature. Emissions factors for fugitive dust are not calculated because PART5 does not properly account for unpaved roads. Newer tools for calculating fugitive dust are available from EPA.

Since MOBILE6.2's release in 2001, there have been three studies sponsored to evaluate the model: one by the Coordinating Research Council (CRC), EPA, and LADCO; a second by the American Association of State Highway and Transportation Officials (AASHTO); and a third by the National Oceanic and Atmospheric Administration (NOAA). A review of the PM emission factor estimating algorithms module also is presented. The results of these studies are summarized in the following paragraphs.

The CRC/EPA/LADCO project (CRC, 2004) compared MOBILE6.2 HC, CO, and NO_x emission estimates with various real-world data sources, including tunnel studies, ambient pollutant concentration ratios, emission ratios from remote sensing devices, and heavy-duty vehicle emission data based on chassis dynamometer testing. Compared with tunnel studies at several sites in the 1990s, the CRC/EPA/LADCO study found that MOBILE6.2 results vary with pollutant. MOBILE6.2 overpredicts fleet average emissions, with the overprediction being most pronounced for CO (especially for newer vehicles). Estimates of NO_x emissions most clearly matched the tunnel study data. Compared with ambient data, the HC/NO_x ratios developed from MOBILE6.2 appear to be reasonably accurate, and the CRC/EPA data generally supported the HC deterioration rates in MOBILE6.2.

AASHTO evaluated several components of MOBILE6.2 (Heirigs et al., 2004), including PM and HAP emission factors, assessment of emission factors when compressed natural gas is the fuel, and methods to estimate CO_2. It found that MOBILE6.2 appears to overestimate exhaust PM_{10} emissions from newer (1991 and later) light-duty gasoline vehicles by about a factor of two. For pre-1990 model years, MOBILE6.2 predictions fall within the range of recent test program expected values. The AASHTO study also found that MOBILE6.2 may be underestimating PM_{10} exhaust emissions from heavy-duty diesel trucks. It also notes that MOBILE6 appears to underestimate wintertime PM emissions, possibly because of a lack of temperature corrections for PM emissions. Finally, the study found that MOBILE6.2 brake-wear emission factors likely underestimate brake-wear emissions from the heavier vehicle classes.

NOAA's comparisons of emissions inventories developed using the MOBILE model and inventories developed using a fuel-based approach tend to support three conclusions. First, there is excellent agreement in the total VOC and NO_x emissions. Second, CO estimates developed using MOBILE are about 40% higher than those developed using a fuel-based approach. Third, although the total emissions of the inventories agree well, the MOBILE NO_x inventory attributes a much smaller fraction (approximately a factor of two) to diesel-powered vehicles and a larger fraction to gasoline-powered vehicles (Parrish et al., 2002).

Outside of California, MOBILE6.2 is probably the most widely used emissions factor model for mobile sources in the United States. Although it is not a modal model, it, nevertheless, is the most tested and validated model. With the exception of VMT, the model provides all inputs required by the emissions air quality models. In response to evolving technology and knowledge, EPA currently is developing a successor to MOBILE6.2, which is discussed just below.

2.1.4. Motor Vehicle Emissions Simulator (MOVES)

To keep pace with new analysis needs, modeling approaches, and data, EPA's Office of Transportation and Air Quality developed MOVES2004. MOVES estimates emissions for onroad and nonroad sources, covers a broad range of pollutants, and enables multiple-scale analysis from fine scale to national emission inventory scale. The foundation of the multiscale approach is a common set of modal emission rates disaggregated by driving mode. These modes then are reaggregated based on representative activity data to estimate total emissions at any scale over any driving pattern. The MOVES2004 model uses a binning approach to define modal emissions. Vehicle-specific power and instantaneous speed are used to identify driving modes. This method produces 17 bins that segregate idle and deceleration and splits the remaining cruise and acceleration operation into 15 bins defined by combinations of speed and vehicle-specific power.

MOVES2004 is used to generate national vehicle emissions inventories and projections at the county level for energy consumption and various pollutants from highway vehicles. The model also generates vehicle emission inventories on mesoscale (regional travel) and microscale (individual transportation facilities) levels. MOVES2004 includes the Argonne National Laboratory's Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model to estimate life cycle (i.e., well-to-pump) effects in the estimate of energy consumption and emissions. MOVES2004 also can be used to estimate pollutant emissions from additional mobile sources, such as aircraft, locomotives, and commercial marine activity; nonroad mobile source emissions; and criteria pollutant emissions.

MOVES2004 has an option of using default data for estimating energy consumption, nitrous oxides, and methane from highway vehicles on a national basis. Detailed information on the inputs for the MOVES2004 model is available in its user's guide (U.S. EPA, 2004). Inputs include selection of scale (macroscale, mesoscale, and microscale), although mesoscale and microscale options are not currently available; selection of geographic bounds for macroscale (nation, State, or county); selection of time spans (year, month, day, or hour); selection of vehicles or equipment (fuels and source use types); selection of road type (off-network, rural interstate, rural local, rural major collector, rural minor arterial, urban collector, etc.); and selection of pollutants and processes (current pollutants include methane and nitrous oxide, and processes include extended idle exhaust, running exhaust, start exhaust, and well-to-pump).

MOVES2004 is written in Java and the MySQL relational database management system. Principal user inputs and outputs and several of the internal working storage locations are MySQL databases. A default input database covering 3,222 U.S. counties is included. MOVES2004 interfaces with a version of the GREET model, which is a multidimensional Microsoft Excel spreadsheet.

MOVES2004 has a master-worker program architecture that enables multiple computers to work together on a single model run. A single computer can be used to execute MOVES2004 runs by installing both the master and worker components on the same computer.

It is not necessary to create a detailed input file for MOVES2004 (unlike MOBILE6), and it is a modal model. These two attributes should make this a user-friendly and attractive model once it becomes fully operational and functional.

Perhaps the single most important weakness of MOVES2004 is that it only models nitrous oxide and methane; therefore, it currently is not possible to model other criteria pollutants such as PM, NOx, gaseous HCs, and CO. This limitation will be corrected with the introduction of a new version, MOVES Highway Vehicle Implementation (MOVES-HVI). A demonstration model is available to the general public. MOVES-HVI can be used to estimate national inventories and projections at the county level for energy consumption (total, petroleum-based, and fossil-based), nitrous oxide, and methane from highway vehicles. The MOVES-HVI demonstration model also performs runs for HC, CO, and NO_x.

2.2. Research-Grade and European Emission Models

These models are included here as they offer features that may benefit specific studies and may be incorporated into future operational-grade emission models.

The Comprehensive Modal Emissions Model (CMEM) is a modal model developed to accurately relate light-duty vehicles emissions as a function of the vehicle's operating mode. CMEM was developed initially using MATLAB, and two command-line interface executables were created for light-duty gasoline and heavy-duty diesel vehicles. Data input is handled via a Java-based graphical user interface (GUI). The model is comprehensive in the sense that it is able to predict emissions for a wide variety of light-duty vehicles in various states of condition (e.g., properly functioning, deteriorated, malfunctioning). The model can predict second-by-second tailpipe (and engine-out) emissions and fuel consumption for a wide range of vehicle and technology categories. The principal strength of this model is that it predicts vehicle emissions modally and is easy to set up and use because of its Java-based GUI. The model is also transparent, and results are easily dissected for evaluation. Because CMEM is not restricted to steady-state emission events, the transient operation of vehicles can be modeled more appropriately. Potential weaknesses with CMEM are the lack of updates for heavy-duty vehicles. Because of its intensive data requirements, CMEM should be considered a research-grade model.

The "COPERT" suite of models was developed for use in Europe by the European Environment Agency (2000). The model, developed using Microsoft Access, is based on methodologies from the European Monitoring and Evaluation Program of long-range transmission of air pollutants and the Core Inventory of Air Emissions. COPERT was designed to produce annual national emission inventories for on- and offroad mobile sources. The latest version, COPERTIV, became available in late 2006. Many of the inputs are Europe-specific and probably not applicable to the United States. Inputs for a typical COPERT run include (1) country fuel, (2) country monthly temperatures, (3) country Reid vapor pressure, (4) country cold-start parameters, (5) activity data fleet information, (6) activity data circulation information, and (7) activity data evaporation share. Outputs from COPERT include the calculation of annual emissions of pollutants for all CORINAIR road traffic source categories at all defined territorial units and road classes. Pollutants include exhaust emissions of CO, NO_x, VOCs, CH_4, CO_2, nitrous oxide, NH_3, sulfur oxides, diesel exhaust particulates (PM), polycyclic aromatic hydrocarbons (PAHs), and persistent organic pollutants, dioxins, furans, and heavy metals contained in the fuel (lead, cadmium, copper, chromium, nickel, selenium, and zinc). Nonmethane VOCs are split into alkanes, alkenes, alkynes, aldehydes, ketones, and aromatics. Although it may be possible to customize COPERT for use in the United States, that probably would be too time and data intensive for most operational applications.

MicroFac is a research-grade emissions model developed by Dr. Rakesh Singh with assistance from EPA. The main application of MicroFac is to provide input to air quality models and emission estimates at small-temporal and fine-spatial scales. According to the model's developer, MicroFac is suited ideally for street-level air quality modeling, identification of hot spots, human exposure assessments, and project-level analysis. The algorithm used in MicroFac disaggregates emissions based on the onroad vehicle fleet and calculates emission rates from a real-time site-specific fleet. MicroFac starts with geographically resolved data, for example, modeling a traffic fleet on an individual length of road. Emission factors are calculated for site-specific on-road traffic fleets (e.g., CO emissions in grams per vehicle kilometers traveled). Total emissions for a geographical area of interest can then be obtained by summing contributions from individual road segments. This approach provides for a shorter and more accurate averaging time, such as a single road during a specific hour of the day. MicroFac requires input variables that are necessary to characterize the site-specific real-time fleet. Input variables required to run the model include date and time, average fleet speed, ambient temperature and relative humidity, road gradient, gasoline fuel properties (such as density, sulfur content, volatility, aromatics, oxygen, olefins, fuel distillation, and heavy metals content), diesel fuel properties (such as density, sulfur, Reid vapor pressure, cetane number, PAH content, volatility, and heavy metals content), length of trip (which is used to calculate the fraction of distance traveled with cold running emissions), and vehicle fleet composition (such as age distribution and percentage of high emitters). In a comparison to MOBILE, Singh and Sloan (2006) suggest that MicroFac is more appropriate than MOBILE for estimating site-specific emission rates from onroad vehicle fleets. An integrated MicroFac and CALINE4 modeling system has been used successfully to calculate vehicle-generated contributions to $PM_{2.5}$ emissions in Canada. However, the model developer has indicated that there is currently not an easy way of writing an input file for MicroFac; it would require the model developer up to 4 days to create an input file for a specific application. Furthermore, according to the developer, the model is still in a research and development phase, although a working model, which is a series of spreadsheets, is said to be available. It is our opinion that MicroFac will require more development and the availability of a user's guide before it is truly operational.

The Mobile Emissions Assessment System for Urban and Regional Evaluation (MEASURE) Model, which was developed with EPA's assistance by the Georgia Institute of Technology, interfaces with a travel demand model output in an ARC/INFO environment to determine emissions on a spatial basis. MEASURE is a research-grade modal model that was developed in the late 1990s. Perhaps the greatest strength of MEASURE is that it can display results graphically using ARC/INFO. ARC/INFO also allows users to define specific areas, thereby allowing modeling at a very fine scale. Because MEASURE is a modal model, it can provide emission estimates for vehicles at multiple speeds or operational modes. The model is further refined by its ability to use socioeconomic data to estimate differences in vehicle fleet by geographic area. This feature is significant because a neighborhood with older vehicles may have higher levels of emissions, which may, in turn, affect geographic patterns of pollutants such as ozone. MEASURE is supported by technical documentation (U.S. EPA, 1998), including a demonstration test case for Atlanta, GA. For this example, a substantial amount of annual data were needed: Georgia Department of Motor Vehicles Registration Dataset, U.S. Census Summary Tape File 3a, U.S. Census TIGER file, Updated TIGER Road Database, Atlanta Regional Commission's (ARC) Traffic Analysis Zones, ARC's Travel Demand Forecasting Network, ARC's Land Use Data, and ARC's ARCMAP Road Database. MEASURE was developed based on statistical distributions of a variety of vehicle technologies and vehicle operating modes. The core of the emission rate model relies on hierarchical tree-based regression analyses. MEASURE is quite modular and includes 11 different interlinking modules, such as road environments, engine start activity, and road activity. MEASURE predicts emissions of CO, HC, and NO_x with a spatial resolution determined by the user (e.g., grams per kilometer or mile traveled). MEASURE does not include nonautomobiles, emission estimates for PM, evaporative emission estimates, effects of vehicle deterioration, effects of grade on engine and accessory load, and intersection specific estimates. Although speed-corrected emission factors from the now-obsolete MOBILE5a model are used, they could be updated easily. For operational use, MEASURE would have to be updated with the latest version of MOBILE and ARC/INFO software. Presumably, this is not an inexpensive task, and the validation of this updated software also could be time consuming.

The Transportation Analysis Simulation System (TRANSIMS) is actually an integrated system of travel forecasting models designed to give transportation planners accurate and complete information on traffic impacts, congestion, and pollution.

TRANSIMS was developed at Los Alamos National Laboratory (LANL) with funding from the U.S. Department of Transportation, EPA, and the U.S. Department of Energy as part of the Travel Model Improvement Program. TRANSIMS simulates the movement of travelers and vehicles across the transportation network in a metropolitan area using multiple modes, including car, transit, truck, bike, and walk, on a second-by-second basis. This virtual world of travelers attempts to mimic the traveling and driving behavior of real people in the region. The interactions of individual vehicles produce realistic traffic dynamics from which analysts can judge the overall performance of the transportation system and estimate vehicle emissions. The Emissions Estimator module requires information from various other modules that are part of TRANSIMS. For example, it needs information from the Traffic Microsimulator. Output from the Emissions Estimator is aggregated on 30-m segments for a 1-h period. The Emissions Estimator module is designed to produce fleet average emissions rather than emissions from individual vehicles. The Emissions Estimator requires information on fleet composition, vehicle loads, and traffic patterns. The TRANSIMS Emissions Estimator module is divided into three submodules: tailpipe emissions from light- and heavy-duty vehicles, and evaporative emissions. For light-duty vehicles, TRANSIMS uses the Comprehensive Modal Emissions Model (CMEM) described earlier). Evaporative emissions are calculated using algorithms that closely follow MOBILE6. Noncommercial users can download Linux-based versions of TRANSIMS for an approximately $1,000 licensing fee. However, commercial users are required to contact IBM. Because of its intensive data requirements, TRANSIMS is currently considered a research-grade emissions model.

3. DISPERSION MODELS

Several review papers on dispersion of vehicular exhaust have been written over the last several years. These review papers cover a variety of model types and methodologies, including Gaussian plume models, puff models, box models, statistical modeling, computational fluid dynamics (CFD), geographical information systems (GIS), and wind tunnel simulations. In addition to the discussions, the review papers also provide an extensive bibliography of research and applications of dispersion models and modeling techniques.

Holmes and Morawska (2006) reviewed the suitability of nearly 30 models for estimating the dispersion of particles, several of which are included in this review. Sharma et al. (2004) reviewed general Gaussian-based highway models (such as CALINE-4 and ROADWAY), dispersion modeling in an urban environment (street canyons and intersections), and recent modeling trends, such as statistical modeling tools, GIS, and, CFD. They also discussed the current status of modeling in India and the routine use of existing line-source models (e.g., CALINE). Vardoulakis et al. (2003) discussed air flow and pollutant dispersion in street canyons, followed by discussions of several operational and research models, model input requirements, and field studies. Nagendra and Khare (2002) presented theoretical considerations of line-source emission models. They reviewed current line-source deterministic models (e.g., CALINE-4), numerical models, and stochastic models. They also presented a short discussion of artificial neural networks as applied to line-source models and discussed some of the limitations of line-source models. The review by Sharma and Khare (2001) is similar in nature to several of the review papers identified above.

The focus of this effort is on Gaussian plume models and puff models. However, a brief discussion of other methods is presented before presenting details on emissions models and dispersion models.

Statistical modeling of air pollution can be carried out by relating meteorological parameters and other parameters after developing a relationship between those parameters and pollutant concentration estimates. Techniques include regression, time series analysis (e.g., Box-Jenkins methods), Markov chain-Monte Carlo methods, and extreme value theory. Gokhale and Khare (2004) reviewed deterministic, stochastic, and hybrid methods of modeling vehicular exhaust. Gokhale and Khare (2005) developed a hybrid model that combined a general finite line-source model (a deterministic model) with a log-logistic distribution model (statistical model) to predict CO from vehicular exhaust. In more recent studies, tools such as artificial neural networks (Nagendra and Khare, 2004) and fuzzy logic theory are being applied to modeling vehicular pollution.

With the increase in affordable computing power, the CFD field has become more popular for dispersion modeling, with the emphasis on the application of CFD techniques on urban street canyons. CFD techniques allow for a more detailed examination of air flow and pollutant dispersion and vehicle-induced turbulence in areas with complex street canyon geometries. Sahlodin et al. (2007) developed a mathematical model that incorporated vehicle-induced turbulence into a Gaussian dispersion model using CFD to simulate the roadway to modify the dispersion parameters. Li et al. (2006) reviewed recent progress in dispersion modeling within urban street canyons in this rapidly developing field.

There are two types of CFD techniques: (1) diagnostic and (2) prognostic. Diagnostic techniques are basically interpolation methods based on measurements that are subject to physical constraints (Li et al., 2006). CFD prognostic techniques can be categorized in three ways: (1) Reynolds-averaged Navier-Stokes (RANS) theory, (2) direct numerical simulation (DNS), and (3) large eddy simulation (LES). The most common RANS techniques are k-ε turbulence closure and renormalized group. These techniques are the least computationally intensive of the three categories and can be used to investigate street aspect ratio, building configurations, inflow (at the top of the building canopy), and vehicle induced turbulence. Sharma et al. (2004) and Li et al. (2006) suggest that some uncertainty exists in the ability of RANS models to simulate urban street canyon pollution problems and, therefore, are more appropriate as a screening approach. DNS methods are the most computationally intensive because the "complete turbulent flow field is solved directly without any form of time or length averaging in the domain" (http://www.fluent.com/elearning/resources/index-glossary.htm). Between the two are large eddy simulation methods that include subgrid scales to model energy-carrying turbulent motions. LES models are more appropriate if speed is of less concern, and the goal is to investigate transient processes and turbulence fields. Huber (2006) presents a framework in which fine-scale CFD modeling may complement a regional modeling system to support human exposure assessments.

Another method of estimating concentrations resulting from vehicular emissions is to use a GIS to map traffic-related pollution. Although GIS does not calculate the impacts resulting from vehicular emissions, it can provide an integrated framework that relates traffic data, emissions, and other related parameters to asses the impacts estimated by a dispersion model. For example, Medina et al. (1994) integrated computer-aided design and drafting (CADD)-based roadway configurations using GIS and traffic information to produce a database appropriate for use in air dispersion models. Gualtieri and Tartaglia (1998) developed a comprehensive approach that includes traffic, emissions, and dispersion modules. GIS can output coordinates of sensitive receptors for input to a dispersion model. Similarly, output from a dispersion model can be input into GIS to display hot spots. Hallmark and O'Neill (1995) developed a model that combines a transportation-based GIS with CAL3QHC estimates. They also discussed problems that arise when transferring data between air quality models and GISs. Sharma et al. (2003) reviewed several approaches that have appeared in the literature and describe a case study in India in which the impacts estimated from CALINE-4 were integrated into a GIS specific for transportation problems.

Another area where research has focused is wind tunnel simulations. These simulations are primarily studies of urban street canyons and intersections and provide insight into the complex flows introduced by the presence of buildings, walls, and vegetation and the dispersion of pollutants. Unlike field observations in which there is little or no control over the meteorological and traffic parameters, wind tunnel experiments provide a controlled environment. Parameters can be held constant or changed to examine the effect on dispersion. Ahmad et al. (2005) reviewed the current state of wind tunnel simulations of the urban environment.

The models presented in this review are primarily Gaussian plume and puff models. A limited number of CFD models and research-based models that are not readily available for public use or review also are presented. Both older and more recent models that can be used to estimate near-roadway pollutant concentrations were identified. This review presents four categories of dispersion models for near-road applications: (1) EPA-recommended models acceptable for regulatory applications, (2) other models freely available to the public, (3) miscellaneous research-grade models, and (4) proprietary models. The model names, model developers, and reference Web sites are listed in Table 3.

3.1. EPA Recommended Models

3.1.1. American Meteorological Society/EPA Regulatory Model (AERMOD)

AERMOD is a steady-state Gaussian plume model released by EPA that replaced the Industrial Source Complex Short Term (ISCST) model in 2006 as a "guideline" model (Cimorelli et. al., 2005). It is used for evaluating the dispersion of inert pollutants from point, area, volume, and open pit sources. If a roadway is simulated as multiple area or volume sources, a single set of coordinates defines the location of each source. AERMOD is designed for transport distance of 50 km or less. AERMOD includes a photochemical option for nitrogen dioxide (NO_2) that accounts for the transformation of NO_2 to nitric oxide (NO) in the presence of ozone, as well as dry and wet deposition options.

AERMOD has a large number of input requirements and requires running a meteorological preprocessor (AERMET) and a terrain preprocessor (AERMAP), assuming local terrain is elevated. There are many commercially available GISs to easily develop the necessary inputs for AERMOD and its associated preprocessors. One of the basic inputs to AERMOD is the control setup file, which contains the selected modeling options, as well as source location and parameter data, receptor locations, meteorological data file specifications, and output options. Another type of basic input data needed to run the model is meteorological data. AERMOD uses state-of-the-art boundary layer parameterizations, and it can utilize site-specific data in its representation of the vertical structure of the atmosphere. AERMOD requires two types of meteorological data files that are provided by the AERMET meteorological preprocessor program. One file consists of surface scalar parameters, and the other consists of vertical profiles of meteorological data. For applications involving elevated terrain effects, the receptor and terrain data will need to be processed by the AERMAP terrain preprocessing program before input to the AERMOD model. Further inputs to AERMOD include the emissions rate per source. The emission rates can be varied by hour of day, but apply to the roadway and not to individual vehicles. The number of receptors, discrete or gridded, is not limited in AERMOD.

AERMOD has an urban option to model urban areas (heat island effects) and provides the capability of specifying sources as urban sources. Because AERMOD is a steady-state model, it does not estimate concentration impacts when the winds are calm. AERMOD includes a meander component that enhances lateral dispersion. Meander is the slow back and forth shifting of the plume and is currently applicable to all but the area sources. AERMOD estimates the

Table 3. Summary of Dispersion Models

Model Name	Developer	URL
	U.S. EPA Regulatory Models	
AMS/EPA Regulatory Model (AERMOD)	U.S. EPA, AMS	http://www.epa.gov/scram001/dispersion_prefrec.htm
CALINE-4	California Department of Transportation	http://www.dot.ca.gov/hq/env/air/index.htm
CAL3QHC/CAL3QHCR	U.S. EPA	http://www.epa.gov/scram001/dispersion_prefrec.htm#cal3qhc
California Puff Model (CALPUFF)	Sigma Research Corporation/ TRC Environmental Corporation	http://src.com/calpuff/calpuff1.htm
	Miscellaneous Publicly Available Models	
Canyon Plume Box Model, version 3.6a (CPB3)	Federal Highway Administration	http://www.tfhrc.gov/structur/pubs/02036/intro.htm
Contaminants in the Air from a Road-Finnish Meteorological Institute (CAR-FMI)	Finnish Meteorological Institute	http://www.fmi.fi/research_air/air_14.html
Emissions and Dispersion Modeling System (EDMS)	Federal Aviation Administration	http://www.faa.gov/about/office_org/headquarters_offices/aep/models/edms_model/
Hybrid Roadway Model (HYROAD)	SAI/ICF Consulting, Inc.	http://www.epa.gov/scram001/dispersion_alt.htm
Point, Area, Line (PAL)	U.S. EPA	http://www.epa.gov/scram001/models/other/altmodel.pdf
Quick Urban & Industrial Complex (QUIC)	Los Alamos National Laboratory in collaboration with the University of Utah and the University of Oklahoma	http://www.lanl.gov/projects/quic/index.shtml
Atmospheric Dispersion Modeling System (ADMS)-ROADS	Cambridge Environmental Research Consultants (CERC)	www.cerc.co.uk/software/admsroads.htm Cost: Approximately $3,700 (annual, single user)
Operational Street Pollution Model (OSPM)	National Environmental Research Institute of Denmark	http://www2.dmu.dk/1_viden/2_Miljoe-tilstand/3_luft/4_spredningsmodeller/5_OSPM/5_description/default_en.asp Cost: Approximately $2,700
PROKAS	Lohmeyer Consulting Engineers, Inc. (German firm)	http://www.lohmeyer.de/air-eia/models/prokas.htm Cost: Approximately $1,876 for PROKAS_B and $4,020 for PROKAS_V

Table 3. Summary of Dispersion Models (cont'd.)

Model Name	Developer	URL
Miscellaneous Research-Grade Models		
Micro-Calgrid Model (MCG)	R. Stern and R. Yamartino	http://www.ivu-umwelt.de/front_content.php?idcat=5
ROADWAY-2	NOAA Air Resources Laboratory	http://www.springerlink.com/index/N07515J23R1T6584.pdf
PUFFER	University of Nottingham (UK)	http://linkinghub.elsevier.com/retrieve/pii/S0167610500000611
TRAQSIM	University of Central Florida	http://cee.ucf.edu/labs/air_quality/SoftwareMain.html
UCD 2001	University of California, Davis	http://pubs.its.ucdavis.edu/publication_detail.php?id=243

effect of meander on concentration estimates by interpolating between two concentration limits: (1) a coherent plume limit and (2) a random plume limit.

As a regulatory model, AERMOD was evaluated extensively using observational field data and tracer study results. A total of 17 databases were used in the evaluation of AERMOD to provide diagnostic as well as descriptive information about the model performance (U.S. EPA, 2003). Also, AERMOD was evaluated with respect to other models such as ADMS-Roads, ISCST3, and CTDMPLUS. When considering only the highest predicted and observed concentrations, it was found that ISCST3 overpredicts by a factor of seven, on average, whereas ADMS-Roads and AERMOD underpredicted, on average, by about 20%. It also was determined that ADMS-Roads performance is slightly better than AERMOD (Hanna et al., 1999). In complex terrain, AERMOD consistently produced lower regulatory design concentrations than ISCST3, not an unexpected result because ISCST3 uses algorithms from a screening model (COMPLEX1) in its calculations. In comparisons with CTDMPLUS and observed data, AERMOD consistently performed better than CTDMPLUS, a model approved by EPA for regulatory applications in complex terrain. The model has not been compared rigorously for line-source applications. Because AERMOD is used most commonly for dispersion analyses of stationary point sources, area sources, and volume sources, there is no accommodation for different roadway geometries (e.g., bridges and deep roadway cuts).

AERMOD also is used as a part of the Emissions and Dispersion Modeling System (EDMS) developed by the U.S. Federal Aviation Administration for assessing the impacts of various emission sources at airports (FAA, 2007). EDMS is EPA's preferred guideline model for modeling dispersion at civilian airports and military air bases (www.faa.gov/about/office_org/headquarters_offices/aep/models/edms_model/).

3.1.2. CALINE-4

CALINE-4 is a Gaussian plume dispersion model that employs a mixing zone concept to roadway sources. This version updates CALINE-3, specifically by fine-tuning the Gaussian method and the mixing zone model. CALINE-4 can model roadways at-grade, depressed, and filled (elevated); bridges (flow under roadway); parking lots; and intersections. Bluffs and canyons (topographical or street) also can be simulated.

CALINE-4 accepts composite vehicle emission factors (expressed in grams per vehicle) developed and input by the user for each roadway link. The user inputs composite emission factors by link. For intersections, the required input parameters are the average number of vehicles per cycle per lane, the average number of vehicles delayed per cycle per lane, hourly departure traffic volume, composite idle emission factor, vehicle idle time at stop line, and vehicle idle time at end of queue. Users also enter hourly information on traffic/sources by link. If a user is modeling an intersection, information on acceleration/deceleration and distance from link end point to the stop line is required. Additional inputs include wind direction bearing, wind speed, atmospheric stability class, mixing height, wind direction standard deviation, and temperature.

CALINE-4 is a Gaussian model whose formulations are based on steady-state horizontally homogenous conditions. The region directly over the highway is treated as a zone of uniform emissions and turbulence. An area equal to the traveled roadway plus 3 m on each side is referred to as the mixing zone. Mechanical turbulence (from moving vehicles) and thermal turbulence (from vehicle exhausts) are the dominant dispersive mechanisms. A modified version of the Pasquill-Smith curves is used for the vertical dispersion coefficient, σ_z. The vertical dispersion parameter is assumed constant over the mixing zone from the center of the roadway link to a computed distance from the link center and then follows a power curve outside this distance. Dispersion is adjusted for vehicular heat flux and surface roughness, which is assumed to be fairly uniform over the study area. The horizontal dispersion is a function of the horizontal standard deviation of the wind direction, downwind distance, diffusion time, and Lagrangian time scale.

CALINE-4 divides highway links into a series of smaller elements. Each element is modeled as an equivalent finite line source (FLS) positioned perpendicular to the wind direction. Each element is subdivided into three subelements to distribute the emissions. The downwind concentrations from an element are modeled using the crosswind FLS Gaussian formulation. The concentration at individual receptors is a series of incremental contributions from each element FLS. The number of receptors that can be modeled by CALINE-4 is limited to 20, making it difficult to compare results to other models that can handle many more receptor locations. The control file is more involved if more than a few days or hours are modeled because the meteorology and vehicular information alternate records in the control file. In addition, there is no meteorological processor available to develop the necessary inputs for 1996 and later.

CALINE-4 is an older model with 1980s science. It is a plume model with steady state, homogeneous conditions. The roadway links cannot be more than 10 m above or below local topography. When compared to measured data, CALINE-4 results show a lower correlation than ADMS-Roads, and best fits lines are also closer to the target line for ADMS-Roads than for CALINE-4. Finally, CALINE-4 has been shown to have a tendency to overpredict low concentrations and underpredict high concentrations of pollutants (Ellis et al., 2001).

3.1.3. CAL3QHC/CAL3QHCR

CAL3QHC is a line-source model used to estimate CO, other inert pollutants, and PM from motor vehicles at signalized intersections. It includes the CALINE-3 line-source model to estimate dispersion using worst-case screening meteorology. CAL3QHC includes methods to estimate queue lengths and emissions from idling vehicles at intersections. CAL3QHCR is a refined model that uses observed meteorological data rather than screening meteorology. In addition, calm winds are excluded in multihour concentration estimates.

These models require a number of detailed inputs, including meteorological variables, deposition velocities, roadway coordinates and dimensions, receptor coordinates, traffic variables (such as traffic volume and speed by link, signal times, clearance time, saturation flow time, and arrival time), and emissions (composite running and idling factors by link).

The dispersion component used in CAL3QHC is CALINE-3, a line-source dispersion model developed by the California Department of Transportation. CALINE-3 estimates air pollutant concentrations resulting from moving vehicles on a roadway based on the assumptions that pollutants emitted from motor vehicles traveling along a segment of roadway can be represented as a “line source” of emissions, and that pollutants will disperse in a Gaussian distribution from a defined “mixing zone” over the roadway being modeled. CAL3QHC/CAL3QHCR only simulates dispersion near intersections for roads that are less than 10 m above grade.

3.1.4. California Puff Model (CALPUFF)

CALPUFF is a non-steady-state Lagrangian model that simulates pollutant releases as a series of continuous puffs and is most suitable for releases in the 50- to 200-km range. It has been adopted by EPA as the preferred model for assessing long-range transport of pollutants and their impacts on Class I areas and on a case-by-case basis for certain near-field applications involving complex meteorological conditions. It can model line sources with constant emissions, as well as point, area, and volume sources.

The inputs for the CALPUFF modeling system can be created either through the GUI available on the CALPUFF download page or through the use of an American Standard Code for Information Interchange (ASCII) text editor.

A meteorological preprocessor (CALMET) generates gridded 3-D diagnostic fields of the winds. An initial-guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce an initial wind field. An objective analysis procedure then utilizes any observational data to refine the winds. The model generates gridded fields of spatially varying fields of temperature, mixing heights, friction velocity, and other boundary layer scaling parameters. Profiles of vertically and horizontally varying turbulence rates also are computed. To estimate turbulence, CALPUFF can use measured values, micrometeorologically scaled parameters from CALMET, or Pasquill-Gifford dispersion coefficients. The dispersion parameters are a continuous function of height that responds to changes in the underlying surface characteristics. A puff-splitting option is available to simulate the effects of vertical wind shear.

CALPUFF can use the full meteorology generated by CALMET, or it can be run in a screening mode using the same input meteorology that is input to the ISCST model.

The CALPUFF developers (http://www.src.com/calpuff/calpuff1.htm)) indicate that CALPUFF may be suitable for the following applications: near-field impacts in complex flow or dispersion situations; long-range transport; visibility assessments and Class I area impact studies; criteria pollutant modeling, including application to SIP development; secondary pollutant formation and PM modeling; and buoyant area and line sources. The developer of CALPUFF makes the model available free of charge with the signing of an end-user license agreement.

A potential weakness of CALPUFF may be that it assumes hourly (or longer) averaging periods and is designed primarily for long-range transport (receptors more than 1 km from a source. Therefore, it may not be ideally suited for modeling near-roadway pollution dispersion.

3.2. Miscellaneous Publicly Available Models

So-called miscellaneous models are freely available to the user community and may be applicable for operational use.

3.2.1. Canyon Plume Box Model, version 3.6a (CPB3)

CPB3 is designed to simulate mobile source impacts within an urban street canyon and narrow highway cut sections (where the surrounding topography is above the level of the roadway) for complex site geometries. The model was developed under the auspices of the Federal Highway Administration (FHWA). The current version of the model is 3.6a. The model can handle a variety of canyon geometries (width to height) and has been tested ranging from about 1:4 to 6:1.

CPB3 requires two input files to run. The first specifies the constants of the application, and the second specifies the variables of the model run. The input constants include street heading, number of lanes, position of lanes, height of vehicles, width of lanes, and number of receptors (from 1 to 20). The input variables include wind speed (miles per second), wind direction (degrees), wind direction standard deviation (degrees), global radiation (kilowatts per square meter), traffic volumes (vehicles per lane per second), traffic speeds (kilometers per hour), emission densities (milligrams per meter per vehicle), observed concentrations (parts per million), and background concentrations (parts per million).

The CPB3 dispersion model is designed to simulate mobile source impacts within urban street canyon or cut-section highway environments. The model can handle a wide variety of canyon/roadway geometries, including curved geometries, one-sided “canyons,” and semipermeable canyons (e.g., semiopen parking garages). The canyon also may be of finite length and terminated at either or both ends with an intersection. Emissions for the model must be provided separately using, for example, the MOBILE emissions model.

The CPB3 research dispersion model is described in the FHWA report, *Modification of Highway Air Pollution Models for Complex Site Geometries* (FHWA, 2002). Although the model can handle a wide range of canyon geometries (e.g., canyon width-to-height ratios from about 6:1 to 1:4 have been tested), it is suggested that the model may have limitations if the application geometry differs appreciably from the simple rectangular notch canyon having a width-to-height ratio of 1. The model developers consider it a research model, rather than a regulatory model, because it is controlled by a great many input variables, and all combinations of these variables in their likely ranges have not been evaluated to the extent "usually expected" for a regulatory model.

Input to CPB3 is relatively simple; only two control files containing time-varying and time-invariant parameters are required. The model was designed to predict pollutant dispersion within a street canyon; therefore, receptors are limited to the canyon environment.

3.2.2. Contaminants in the Air from a Road-Finnish Meteorological Institute (CAR-FMI)

CAR-FMI models an open-road network of finite line-source emissions for inert and reactive ($NO_x$and ozone [O_3]) gases, as well as fine particulates ($PM_{2.5}$) from vehicle exhaust. Dry deposition is included for particulates. There is limited chemistry using the discrete parcel method for CO, NO, NO_2, NO_x, O_3, and $PM_{2.5}$.

CAR-FMI requires inputs that are typical of dispersion models. These include location of line sources, hourly traffic volumes for each road, hourly meteorology, hourly background concentrations, and emission coefficients.

CAR-FMI is a Gaussian plume model. The general analytical solution of Luhar and Patil (1989) (described in Section 3.4 as GFLSM-LP) is used to solve the dispersion of gases. Atmospheric boundary layer theory is used for estimating turbulence parameters. A finite length source algorithm is used to estimate concentrations of inert and NO_x reactive pollutant and fine PM. A Windows-based GUI is available to assist in developing the inputs and running the model.

A limitation to CAR-FMI is that it is only applicable to at-grade or near at-grade roadways. In addition, it currently is not known whether the model code is available. One Web site (http://www.mi.uni-hamburg.de/Car-fmi.336.0.html) indicated that the code was obtainable from the developers, but this could not be verified.

3.2.3. Hybrid Roadway Model (HYROAD)

HYROAD integrates three historically individual modules that simulate the effects of traffic, emissions, and dispersion. The traffic module is a microscale transportation model that simulates individual vehicle movement. The emission module uses speed distributions from the traffic module to determine composite emission factors; spatial and temporal distribution of emissions is based on the vehicle operation simulations. The model tracks vehicle speed and acceleration distributions by signal phase per 10-m roadway segment for use in both emissions distribution and for induced flows and turbulence. The dispersion module uses a Lagrangian puff formulation, along with a gridded nonuniform wind and stability field derived from traffic module outputs, to describe near-roadway dispersion characteristics. HYROAD is designed to determine hourly concentrations of CO or other gas-phase pollutants, PM, and air toxics from vehicle emissions at receptor locations that occur within 500 m of the roadway intersections.

HYROAD requires simplified meteorological inputs: wind speed and direction, standard deviation of the horizontal wind speed, Pasquill-Gifford stability class, a mixing height, and ambient temperature. An ambient background concentration also can be entered. Multiple dispersion scenarios can be run to simulate multiple hour simulations.

The model uses a Gaussian puff approach in which dispersion processes are affected by vehicle wakes. Methods developed by EPA and incorporated into EPA's ROADWAY model (in the mid-1980s), as well as some of the puff formulations from CALPUFF are adapted into HYROAD. The module creates a 2-D nonuniform wind field that advects the puffs and enhances vertical dispersion over the roadway.

HYROAD is a single package with traffic, emissions, and dispersion components contained in a single GUI. HYROAD is primarily an intersection model, but can simulate a highway link by creating a very long link between intersections (on and off ramps). The traffic module of HYROAD appears to run only under Microsoft Windows 98. To run the complete package requires installing software that emulates the Windows 98 operating system; therefore, HYROAD may not be the best option for near-roadway applications.

3.2.4. Point, Area, Line (PAL)

PAL is a multisource steady-state Gaussian plume model for nonreactive gaseous and suspended particulate pollutants. Developed in the 1980s, its application is primarily at the urban microscale environment (up to several hundred meters) and is included here for historical perspective. Six source types can be modeled with PAL: point, area, two types of line sources (line and slant line), and two types of curved path sources (curved and special path). The slant line and curved special path sources are for modeling sources in which the end points are at different heights above ground, such as a freeway onramp. Options for dry deposition and gravitational settling are included, but the model does not perform any chemical transformations.

There are 13 input “card” types for PAL that define the program control options, source data, meteorological data, and receptors. Each source’s emission rates are constant, but PAL provides a means to vary the emissions by hour of day for each source type. Options for the diurnal variations of the emissions can be input for each source type for each hour. Up to 99 sources can be entered in a single model run.

Meteorological data include wind direction and speed, wind profile exponents, anemometer height, stability class, mixing height, and ambient air temperature. Winds can vary as a function of height or can be held constant, and the manner in which the wind speed is varied can be specified by source type. PAL can process up to 24 h of meteorology in a single model run.

PAL is a relatively old Gaussian plume model that assumes steady-state conditions and nonvarying winds within the modeling domain, and it does not perform well in low-wind-speed situations. The model does not have any provisions for building downwash and is not appropriate for complex terrain situations.

3.2.5. Quick Urban & Industrial Complex (QUIC)

The QUIC modeling system consists of three “modules:” (1) QUIC-URB, an urban wind model; (2) QUIC-PLUME, a Lagrangian dispersion model; and (3) QUIC-GUI, a GUI. The QUIC system was developed to calculate wind and concentration fields in cities with complex clusters of buildings. It is a diagnostic-empirical system that accounts for building-induced circulations. This type of model is not nearly as computationally intensive as CFD models, which also are used to simulate dispersion and transport in cities.

The QUIC-URB wind model is based on a mass-consistent diagnostic wind model that computes the 3-D flow field around buildings. In QUIC-URB, an initial wind field is prescribed with flow effects associated with the buildings superimposed on it. Empirical algorithms are used to determine the initial wind field at rooftops and upstream recirculation zones, in the downwind cavity and the wake of a single building, and in the street canyons between buildings. The final flow field is solved by ensuring mass conservation.

The QUIC-PLUME dispersion model tracks the movement of individual particles using the mean wind field calculated by QUIC-URB and produces the turbulent dispersion using random-walk equations. Additional drift terms are included to account for the heterogeneous nature of turbulence around the various buildings. Gradient transport and similarity theory are used to estimate normal and shear stresses and the turbulent dissipation. QUIC-PLUME includes a nonlocal mixing formulation to better describe the turbulent mixing in building cavities and wakes. In their modeling using QUIC, Kastner-Klein and Clark (2004) implemented a vehicle-induced turbulence (they use the term traffic-produced turbulence) parameterization into QUIC-PLUME.

Although not as accurate as a CFD model, the QUIC model captures major flow features with significantly less computational resources. The model has been validated against wind tunnel experiments, observational field experiments (Salt Lake City URBAN 2000 Tracer Experiment [Gowhardhan et al., 2006]), and other models (e.g., FLUENT) with promising results. The model also comes with a GUI that makes running the model easier for the user.

The model and documentation are not readily available to the general public. Several documents at LANL on the QUIC system, including PLUME theoretical formulation and user's guides, are "at scanning," according to the LANL Web site.

3.3. Proprietary Models

This class of models, although possessing many advanced features, currently must be purchased. Because they possess features and capabilities not included in the other models, they are included in this section.

3.3.1. Atmospheric Dispersion Modeling System (ADMS)-Roads

ADMS-Roads is a "comprehensive tool for investigating air pollution problems because of small networks of roads that may be in combination with industrial sites" (McHugh et al., 1997). Roadway and industrial sources (point, area, and volume) can be modeled together. ADMS-Roads includes a chemistry module for NO_x-to-NO_2 conversion and sulfate chemistry. A street canyon module based on the Danish Operational Street Pollution Model (OSPM; see Section 3.3.2) is available. A module for dispersion in complex terrain is included. ADMS-Roads also can model the effects of street canyons, noise barriers, and vehicle induced turbulence.

ADMS-Roads requires an extensive number of data inputs: source parameters (including source locations, road widths, building canyon heights, stack heights and diameters, and up to 7,000 road links); meteorological data; hourly traffic flow; emission factors; and background concentrations.

The model's Web site does not contain detailed information on the technical aspects of the model. According to Cambridge Environmental Research Consultants (CERC), the science of ADMS-Roads is significantly more advanced than that of most other air dispersion models (such as CALINE and ISCST3) in that it incorporates the latest understanding of the boundary layer structure and goes beyond the simplistic Pasquill-Gifford stability categories method with explicit calculation of important parameters. The model uses advanced algorithms for the height dependence of wind speed, turbulence, and stability to produce improved predictions. In addition, ADMS-Roads incorporates CERC's FLOWSTAR model to calculate changes in mean flow and turbulence because of terrain and changes in land use. It has links to ArcView and MapInfo GIS packages, as well as to the Surfer contour-plotting package. The GIS link can be used to enter and display input data and display output, usually as color contour plots. From the brief discussion on the ADMS-Roads Web site, the technical formulation appears to be similar to that of AERMOD.

Several models were compared to ADMS-Roads for a variety of site conditions (flat/complex terrain and rural/urban). For the highest predicted and observed concentrations, ISCST3 overpredicted by a factor of seven, on average, whereas ADMS-Roads and AERMOD underpredicted, on average, by about 20%. It also was determined that ADMS performance is slightly better than AERMOD (Hanna et al., 1999). A comparison of ADMS-Roads and CALINE-4 with measured concentrations suggested that the ADMS-Roads "line-of-best-fit" is closer to the target line than CALINE-4. Both models tended to overpredict low concentrations and underpredict high concentrations (Ellis et al., 2001).

3.3.2. Operational Street Pollution Model (OSPM)

OSPM is a practical street pollution model that was developed by the National Environmental Research Institute of Denmark. Concentrations of exhaust gases are calculated using a combination of a plume model for the direct contribution and a box model for the recirculating part of the pollutants in the street. The model can be used for streets with irregular buildings or buildings on one side only but is best suited for regular street-canyon configurations. The model should not be used for crossings or for locations far from traffic lanes.

The required input data are hourly values of wind speed, wind direction, temperature, and global radiation. The two last parameters are used for calculation of the chemical transformation of NO-NO_2-O_3. The model also requires hourly values of urban background concentrations of the modeled pollutants. In addition to the hourly input parameters, the model requires data on street geometry and street traffic.

A Microsoft Windows version contains a user-friendly interface that allows for online preparation of all required input data and files. The Windows version, which is distributed under the name WinOSPM, contains special modules for preparation and visualization of traffic data and traffic emissions.

Concentrations of exhaust gases are calculated using a combination of a plume model for the direct contribution and a box model for the recirculating part of the pollutants in the street. It is assumed that both the traffic and emissions are uniformly distributed across the canyon. It also is assumed that the canyon vortex has the shape of a trapezoid, with the maximum length of the upper edge being half of the vortex length. The ventilation of the recirculation zone takes place through the edges of the trapezoid, but the ventilation can be limited by the presence of a downwind building if the building intercepts one of the edges. The concentration in the recirculation zone is calculated assuming that the inflow rate of the pollutants into the recirculation zone is equal to the outflow rate, and that the pollutants are well mixed inside the zone. The turbulence within the canyon is calculated taking into account the traffic-created turbulence. The traffic-induced turbulence plays a crucial role in determining pollution levels in street canyons. During windless conditions, the ambient turbulence vanishes, and the only dispersion mechanism is because of the turbulence created by traffic. Therefore, the traffic-created turbulence becomes the critical factor determining the highest pollution levels in a street canyon.

The model has been used in a number of studies and is well documented. One study concluded that the use of computed urban background concentrations as input values to the OSPM model yields a fairly good agreement with measured data (Wallenius et al., 2001).

3.3.3. PROKAS

PROKAS consists of two modules: PROKAS_V and PROKAS_B. PROKAS_V provides the basic software module, and PROKAS_B provides enhancements to the model (e.g., street canyon capabilities). PROKAS_V is based on the German guideline VDI 3782/1 "Gaussian Dispersion Model for Air Quality Management." Modeling of up to 5,000 line sources (reproduced by sets of point sources) of a network of streets is possible. The model accounts for the traffic-induced turbulence and the influence of noise protection devices for each street.

Input requirements include street coordinates, emissions for up to three pollutants, street-specific dispersion parameters (to account for near-field flow disturbances, such as from traffic-induced turbulence), dispersion parameters, receptor coordinates, background concentrations, hourly emissions, and meteorological statistics (such as 3-D winds and atmospheric stability).

The model was developed according to the German Emission Factors Handbook, coupled with the Gaussian Dispersion Model. The model also has an interface to MOBILEV, a German emission factor model.

PROKAS is not applicable when the wind field is not homogeneous in the area under consideration or in areas with valley drainage flows, when the influences of buildings have to be considered in detail, or at distances less than 10 m from the line source.

3.4. Miscellaneous Research-Grade Models

There are various research-grade dispersion models for near-road applications developed by universities, private companies, and government agencies. In this review, we describe several types of models: Eulerian grid models, puff models, and finite line-source flume models.

The Micro-Calgrid model (MCG) developed by R. Stern and R. Yamartino is a microscale photochemical model for applications in complex urban environments such as street canyons. MCG is a photochemical model that solves Eulerian equations of motion with turbulence closure based on two energy production-dissipation equations, includes detailed treatment of vehicle induced turbulence, and has three chemistry schemes. MCG includes MOBILEV, a traffic-induced emissions model from the German Federal Environmental Agency; MISKAM, a CFD microscale flow model; and MCG, an Eulerian grid model. The starting point for the development of MCG was Calgrid, a second-generation photochemical model with 3-D advection-diffusion for each pollutant species. MCG includes resistance-based dry deposition rates, CBM-IV and SAPRC-93 photochemistry mechanisms, and a chemical integration solver. Micro-Calgrid accounts for vehicle-induced turbulence by considering energy dissipated by a vehicle as it moves through the ambient air. The micrometeorological driver for MCG is MIKSAM, which is a 3-D flow model for inert pollutants. The MIKSAM flow model may not perform well in stagnant or low wind conditions. Emissions data come from the German MOBILEV model. Yearly averages or hourly emissions for on-street or a network of streets are computed from emission factors from the German Federal Environment Agency, street characteristics, traffic activity, and the composition of the vehicle fleet. Because MCG is a street canyon model, it will not be well suited for the generic near-roadway modeling applications.

The ROADWAY-2 model developed by NOAA Air Resources Laboratory (Rao, 2002) is a non-steady-state model that incorporates an atmospheric boundary layer model with turbulent kinetic energy closure and up-to-date surface parameterizations to derive mean and turbulence profiles. ROADWAY-2 is based on EPA's ROADWAY model developed by Eskridge and Catalano (1987). Information on any other user inputs was not obtainable in the absence of a review of the source code. The concentration equations are solved using a fractional-step finite difference method. Vegetation canopy flow theory was used to derive vehicle wake parameterizations. Vehicle wake velocity deficit is proportional to the square of the relative wind speed, and the rate of vehicle wake production of turbulent kinetic energy is proportional to the cube of the relative wind speed. ROADWAY-2 provides an advanced treatment of atmospheric velocity and turbulence fields. The model was evaluated using tracer data from the 1975 General Motors (GM) experiment in Milford, MI. Model predictions were in good agreement with the observed data, with a tendency for slight underprediction for all orientations of the wind to the roadway. For winds parallel to the roadway, which can be difficult to model, ROADWAY-2 again was in good agreement with the GM observations, with a tendency for slight overprediction. The model requires temperature, wind speed, and wind direction from two heights, although it can run with speed and direction from a single height (and temperature from two levels). These data should come from instrumentation located upwind of the roadway, therefore, data routinely available from a single height, such as National Weather Service airport data, are not suitable for this model. Unfortunately, there is no user's guide or manual for this model to assist in developing the necessary input files.

The PUFFER model was developed as part of a doctoral dissertation at the University of Nottingham (UK) to model vehicular pollutants in an urban street canyon. The dispersion is based on Gaussian puff methods but with an extended range of applicability. The model includes the explicit effects of individual vehicles as sources of pollution and turbulence over multiple lanes of traffic. Each vehicle emits a puff at the start of a time step, and each puff maintains its independence of all other puffs (i.e., no consideration for puffs crossing paths). Local air flow is the superposition of the ambient wind and movement of the vehicles. A puff is influenced only by the wake of the vehicle directly in front. Inputs to PUFFER include specifying modeling options, canyon geometry, number of lanes, meteorology (wind speed, angle to canyon axis, roughness length), vehicular data, time step and puff frequency, and selection of output options. In addition, emissions are input as part of the puffer.dat input file. Puffer.dat includes the number of vehicle types; length, width, and height of each vehicle type; velocity control parameter; headway parameters; idling emission rate; speed-dependent emission coefficient; and acceleration-dependent emission coefficient. An advantage of this model is that it is a puff model applied to vehicular emissions. Real-time buildup of traffic can be simulated using the traffic submodule. An inherent weakness is that only 1 h at a time can be modeled. Perhaps the most limiting weakness is that the scripts to set up the model runs have been lost. No updates to PUFFER have been published, and no additional work has been performed on the model since the results were published.

The TRAQSIM model was developed by the University of Central Florida in support of a doctoral dissertation. TRAQSIM is a puff model for flat terrain (i.e., topography is not addressed) that tracks vehicular exhaust released as individual puffs using modal emissions factors from CMEM that were incorporated into a lookup table for TRAQSIM. TRAQSIM combines traffic, emissions and dispersion components into an integrated, graphical framework. TRAQSIM is applicable for emissions of CO and other nonreactive pollutants. TRAQSIM has three modules, each of which has a separate set of inputs that are entered via GUI: (1) Traffic/Sources, (2) Dispersion/ Meteorology, and (3) Emissions. The dispersion module makes use of a Gaussian puff model that tracks discrete moving sources, rather than treating highway sections as line sources. Atmospheric turbulence is modeled as a function of Pasquill-Gifford stability class. In an initial model-to-model validation, Kim et al. (2007) modeled a simple road link and compared results from CAL3QHC and TRAQSIM. They noted that TRAQSIM produced more "intuitively correct" spatial allocation of impacts when compared with CAL3QHC (which used emission factors derived from TRAQSIM). In a second validation, the two models were compared using high-quality field data collected in Denver, CO. A much more complex roadway representation was modeled. The results of this comparison indicate that TRAQSIM performed on par with CAL3QHC. The Visual Basic interface should be considered a prototype as it has various bugs in it that need to be worked out. As the number of puffs increases, the simulation slows considerably because no puffs are removed (although there is an algorithm to merge puffs). A 1-h simulation requires about 25 to 30 min on a 2.8-GHz Pentium desktop computer for a free flow section of about 300 m.

The UCD 2001 dispersion model, developed by the University of California, Davis, is designed to estimate pollutant concentrations near at-grade roadways. The model is intended for use from 3 to 100 m downwind of the edge of a roadway (Held, et al., 2003). The UCD 2001 model was calibrated with one-half of the GM sulfur hexafluoride tracer study database and resulted in a selection of eddy diffusivity parameters that did not vary with ambient meteorology. This parameterization is consistent with several independent studies that indicate that the atmosphere is well mixed and neutrally stratified immediately downwind of a roadway with significant vehicular activity. User input requirements for the UCD 2001 model include roadway and receptor geometry, vehicular data, and meteorology. Because the application of this model is limited to within 100 m of the roadway, and mixing resulting from the motion of the vehicles is intense near roadways, atmospheric stability is ignored. Applications further downwind of a roadway likely would require rethinking some of the model's internal parameters and, possibly, its formulation. It is not known if the model can be run for multiple hours or if it only runs 1 h at a time. The UCD 2001 model is based on the work of Huang (1979) who developed a non-Gaussian model for turbulent shear flow that uses "apparent" lateral diffusivity. UCD 2001 model performance was evaluated and compared with the CALINE3 and CALINE4 dispersion models using the GM database. UCD 2001 adequately simulates near parallel, low-wind-speed (<0.5 m/s) meteorological scenarios, whereas the CALINE models significantly overpredict most receptor concentrations for these conditions. The UCD 2001 model results in approximately 80% to 90% reduction in squared residual error when compared with the CALINE3 and CALINE4 models. In addition, the UCD 2001 model exhibits better agreement in simulating the top 40 observed concentrations than either CALINE model. Lastly, the UCD 2001 model requires less user input and modeler expertise than most roadway dispersion models and should result in more consistent and robust pollutant field estimations. The model is not publicly available, but might be available from the University of California, Davis. It is not known if a user's guide or manual exists for this model.

There are several general finite line-source models described in multiple research papers: Luhar and Patil (1989), Esplin (1995), Venkatram and Horst (2006). Chock (1978) developed an infinite line-source model (referred to as the GM model) to model dispersion from roadways. The GM model overpredicts concentration for upwind roadway segments that are less than three times the perpendicular distance from the roadway to a receptor. Csanady (1972) developed a model for a finite line source, but it was applicable only when the wind was perpendicular to the roadway. Calder (1973) developed an infinite line-source model that was more appropriate for winds at an angle to the roadway.

Luhar and Patil (1989) developed a simple general finite line-source model (hereafter referred to as GFLSM-LP) to overcome constraints imposed by modeling of infinite line sources. According to the authors, the GFLSM-LP can handle all orientations of wind direction relative to a roadway. Esplin (1995) extended Calder's work to a finite line source. However, Esplin reports that the model is not applicable if the wind direction is within 15° of the orientation of the roadway (i.e., nearly parallel to the roadway). Venkatram and Horst (2006) also report that these models perform poorly as the wind direction approaches the orientation of the roadway. None of these models have chemical transformation capabilities.

In these research-grade models, concentration estimates are assumed to follow a generalized Gaussian plume model formulation. The development of the line-source formulation includes a transformation between the line-source coordinate system in the standard east-west and north-south orientation and a wind coordinate system in which the *x* axis is in the direction of the mean wind. In this rotated system, the horizontal and vertical dispersion parameters (σ_y and σ_z) are functions of the downwind distance and may not be known, so they are transformed into forms that are functions of the line-source coordinate system.

In their development, Luhar and Patil (1989) account for the height of the receptor above ground in the Gaussian equation. They also include a ground reflection term, adjust the mean wind speed with a correction for traffic wake effects to account for lateral dispersion when the wind speed approaches zero or the wind direction is nearly parallel to the orientation of the roadway, and incorporate the effects of plume rise in their final form of the line-source model. In both models, their form of the vertical dispersion coefficient introduces a singularity when the wind is parallel to the road. They use expressions from the GM model (Chock, 1978) to avoid this complication. Esplin developed a model that is valid for wind directions from 0° to 75° when the Gaussian plume model is used. In his formulation, he uses a fraction of ground reflection term rather than explicitly included a term in the final equation. This fraction is incorporated into a general term representing all terms that are not dependent on cross-wind distance. Venkatram and Horst (2006) derive a model similar to Esplin (1995), with the main difference being that the limits of integration correspond to downwind distance from the end points of the line segment to the receptor. This results in σ_z being evaluated at an effective distance between the line segment and the receptor in the rotated system but allows σ_y to be evaluated in the unrotated system. Ganguly and Broderick (2006) found that predictions from CALINE-4 and GFLSM-LP are very close to each other and agreed well with monitored data. They found the main advantage of a GFLSM-LP "lies in the simplicity of its application as it is an analytical solution of the Gaussian equation." A sensitivity analysis conducted by Ganguly and Broderick (2006) found that the GFLSM-LP model performs well for neutral conditions but worse for low wind speed conditions. This model performs poorly for winds that are parallel or nearly parallel to a roadway. Validation tests on this model also indicate the model underpredicts PM for all size ranges. Finally, the model is applicable only to CO and other inert pollutants and PM.

Venkatram et al. (2007) developed a dispersion model and used it to analyze measurements made during a field study conducted by EPA in July and August 2006 to estimate the impact of traffic emissions on air quality at distances of tens of meters from an eight-lane highway located in Raleigh, NC. This dispersion model for road emissions can be incorporated readily into the current generation of dispersion models typified by AERMOD (Cimorelli et al., 2005). Unlike CALINE (Benson, 1992), which uses stability-based Pasquill-Gifford dispersion curves, this model requires micrometeorological inputs compatible with those of AERMOD. The most important meteorological input is the standard deviation of the vertical velocity fluctuations. In principle, it can be estimated from the type of measurements customarily required by current models.

4. SUMMARY

This document has described a number of emission and air quality models available for near-road application. The focus has been on models that are operational or that have features that could be incorporated into operational models. Of the emission models listed above, MOBILE6.2 is the most widely used, tested, and accepted model. Although it is not a modal model, it has the best representation of the vehicle fleet in the United States. As a future replacement of MOBILE6.2, EPA is developing MOVES, which will handle modal emissions. In addition to capturing modality in traffic activity patterns, some other future directions are becoming evident. For example, in comparing two emission modeling approaches in Philadelphia, PA, Cook et al. (2006) conclude that more accurate estimates occur when traffic demand model data are used at a link level rather than at an aggregated county level.

With the exception of including the effects of vehicular-induced turbulence, near-road dispersion models have advanced little over the past two decades. Also, the commonly applied dispersion model, AERMOD, contains a very simplistic algorithm for simulating line sources. For a modest investment, near-road air quality models could be upgraded to include a more accurate line-source algorithm and could be modified to account for features such as noise barriers and vegetation, which can perturb near-field ground-level concentrations of air pollutants. Furthermore, field, laboratory, and advanced numerical modeling studies (using models such as CFD and QUIC) could be used to evaluate and parameterize important physical processes that are not captured in existing operational models.

The need for further research on emission and air quality models is further bolstered by recommendations from a 2006 workshop on PM research needs organized by FHWA (McCarthy et al., 2005). Two of the three highest priorities for research are (1) to evaluate "hot spot" air quality models and (2) to develop and to evaluate emissions models. Work on these two priorities arguably would advance the application of near-road emission and air quality models.

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