Development of the Traffic Air Quality Simulation Model (TRAQSIM)

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The United States (US) Environmental Protection Agency (EPA) currently promulgates the use of CAL3QHC to model concentrations of carbon monoxide (CO) near roadway intersections. The steady-state and macroscopic methods used in this model represent rough approximations of the physical phenomena occurring at intersections and are unintuitive for the users. Therefore, the Traffic Air Quality Simulation Model (TRAQSIM) was developed to create a theoretically more realistic (more natural), easier to understand, and more flexible modeling environment than CAL3QHC. Instead of steady-state plume equations used in CAL3QHC, TRAQSIM models dispersion through the use of Gaussian puffs emitted from discrete moving sources in a traffic simulation environment. Although most of the components incorporated in TRAQSIM are not new, the combination of these components within a fully integrated environment is new and provides the potential for more direct (more logical) expansion of modeling capabilities. As part of an initial validation assessment, a relative comparison of CAL3QHC and TRAQSIM results showed that TRAQSIM produced more intuitively correct spatial allocation of concentrations. The validation assessment also showed good agreement by both models when compared to measured data with overall R^2 values of 0.721 for CAL3QHC and 0.605 for TRAQSIM. Although this appears to favor CAL3QHC, analyzing individual cases show mixed results (i.e., 6 cases favoring CAL3QHC and 5 cases favoring TRAQSIM). Therefore, additional assessments with larger datasets will need to be conducted before any definitive conclusions can be made. This paper describes the data and methodologies used to develop TRAQSIM and the initial validation work.

INTRODUCTION

The Environmental Protection Agency (EPA) currently promulgates the use of CAL3QHC for air quality, especially carbon monoxide (CO) concentration, assessments involving interrupted traffic scenarios (e.g., intersections). CAL3QHC represents vehicles as part of line sources in calculating concentrations of relatively inert pollutants (i.e., CO). The average and steady-state characterization of traffic movements, vehicle emission rates, and atmospheric dispersion methods employed by the model present several shortcomings. First, CAL3QHC's use of line sources with evenly distributed emission factors (i.e., uniform density) and the representation of idling (queued) vehicles with equivalent length line sources are homogenous approximations of actual traffic conditions and do not allow accurate modeling of modal activities such as acceleration on departure links. Second, the use of steady-state Gaussian equations for dispersion modeling does not allow the direct use of time-varying meteorological data, and therefore, precludes the direct modeling of time variances. Third, the dispersion effects of vehicle wakes and exhaust gas buoyancy are generically approximated through the use of homogeneous mixing zones that do not reflect the complex interactions between vehicle locations and these dispersive factors. Lastly, CAL3QHC does not account for the drag-effects of vehicle wakes which add to the advection of the pollutants, and thus, their dispersion as well.

Due to these shortcomings, there exists the potential to improve upon CAL3QHC through more realistic representations of the physical phenomena (e.g., vehicle modal movements, wake effects, exhaust buoyancy, etc.) occurring along roadways. A more realistic model could also result in a more robust modeling environment that allows users to model scenarios in a more straightforward or direct manner with less burden on input requirements.

The new model entitled, Traffic Air Quality SImulation Model (TRAQSIM), was developed as part of a Ph.D dissertation at the University of Central Florida [Kim 2004]. The model uses a simulation approach where the movement of each individual vehicle is modeled at an interrupted traffic scenario such as a signalized intersection. Thus, each vehicle is modeled as a discrete moving source with appropriate modal movements (e.g., acceleration, deceleration, etc.) and emissions during each simulation time-step. The emitted pollutants are modeled as a series of Gaussian puffs (i.e., rather than plumes) with one puff being emitted per vehicle for each time-step. Advection of each puff is accomplished through contributions from the mean wind, vehicle wake effects (dragging), and atmospheric rise (e.g., thermal buoyancy) of the vehicle exhaust gases.

A comparable model developed by Systems Applications International (SAI), Inc. under sponsorship by the National Cooperative Highway Research Program (NCHRP) was designed to incorporate traffic simulation with emissions and dispersion models [Carr 2002]. Entitled HYROAD, the relatively new model (Version 1.1) is currently available from EPA and undergoing continued evaluations. Similar to TRAQSIM, all of the computational components within HYROAD are based on existing models. Traffic simulation is handled through the incorporation of the urban Network Simulation (NETSIM) model. For emissions modeling, HYROAD uses average emission factors but for different driving cycles including the Federal Test Procedure (FTP) cycle used in the MOBILE-series models. HYROAD does not use modal emission factors, but may be implemented in a future version [Carr 2002]. Dispersion modeling is accomplished through the use of the CALPUFF model which allows time-varying input data to be used.

Although HYROAD combinex these components into a working model, the components are loosely combined such that they mimic the separate use of each component one at a time rather than an integrated model that uses all components together as a whole. A case in point is that the vehicular sources in HYROAD are not modeled as moving sources as in TRAQSIM; rather, vehicle movements are simulated in order to obtain aggregate-level traffic parameters that are then fed into the emissions and dispersion models. The integration approach used in TRAQSIM also tends to allow for better modeling performance because there are fewer restrictions on the interactions and feedbacks between the modules. A natural outcome of a true integration is that it frees-up the user from having to translate and/or understand the use and effects of the same variable in different modules/models.

MODEL DESCRIPTION

TRAQSIM is composed of three main components: (1) Traffic Simulation; (2) Modal Emissions; and (3) Atmospheric Dispersion. The following sections provide detailed descriptions of these components.

Traffic simulation

The traffic simulation module developed for TRAQSIM was not intended to be a high fidelity model that could compete with widely used existing models. Rather, the goal was simply to develop a module that would provide reasonably realistic movements of vehicles sufficient for air quality analysis. To that end, leader vehicle movements were modeled through the use of simple equations of motion with adherences to signal and stop sign rules. To realistically model driving behaviors, stochastic cruise speeds were assigned to each vehicle and a car-follower algorithm was implemented.

The vehicle types modeled in TRAQSIM are mostly based on types from the University of California at Riverside's (UCR's) Comprehensive Modal Emissions Model (CMEM). TRAQSIM uses all 26 light-duty CMEM vehicle types and adds 5 more based on vehicle types from the MOBILE6 model for a total of 31:

- CMEM: 1-25, 40
- MOBILE6: heavy-duty gas vehicle (HDGV), light-duty diesel vehicle (LDDV), light-duty diesel truck (LDDT), heavy-duty diesel truck (HDDT), and motorcycle (MC)

Each individual vehicle is treated as a discrete moving source (or object) within the simulation environment. As a vehicle is created and enters a link, it possesses the specified cruise speed of the link with some stochastic variation. Therefore, all new vehicles are initially assigned to the cruise mode. The variation is accomplished by randomly selecting from a normal distribution around the specified cruise speed. An arbitrary but reasonable standard deviation of 5 mph is used with caps placed at the 20 and 80 percent levels (i.e., to prevent very large deviations in the assigned speeds). In terms of geometric shape, all vehicles are modeled as one of four types: (1) light-duty vehicle (passenger car and light-duty truck), (2) medium truck, (3) heavy-duty vehicle, or (4) motorcycle. The overall dimensions as well as exhaust heights and their sources are discussed in Kim 2004.

TRAQSIM's movement algorithms are based on two vehicle types: leader and follower. The leader vehicles are only affected by signals and stop signs. With no obstructions, these vehicles always "desire" to attain the cruise mode at their assigned cruise speeds. Since each vehicle's predetermined cruise speed is a cap, there are no conditions under which a vehicle will ever exceed its cruise speed. When a vehicle is at a speed less than its cruise speed and is free to accelerate, it will do so according to the linear relationship shown in Equation 1.

$$a = \text{alpha} - \text{beta}(V) \qquad (1)$$

where a = acceleration rate (m/s^2)
alpha = intercept of linear fit
beta = slope of linear fit

The alpha and beta values were obtained from data in the 1990 "Green Book" by AASHTO, and they represent "design" conditions [AASHTO 1990 and Long 2000]. The deceleration rate of a leader vehicle is modeled using Equation 2.

$$d = - V^2 / 2D \qquad (2)$$

where d = deceleration rate (m/s^2)
V = current speed of vehicle (m/s)
D = distance to stop behind signal, stop sign, or leader vehicle (m)

The distance (D) for a leader vehicle is generally a decision distance (DD) used to determine when a vehicle will "normally" start a deceleration phase. This is represented by Equation 3.

$$DD = 0.218V^2 + 1.188V + 4.425 \qquad (3)$$

where DD = decision distance (m)

Equation 3 was derived through regression analysis ($R^2 = 0.9999$) of data in the Traffic Engineering Handbook [ITE 1999]. The data was regressed because for model implementation purposes, it was deemed easier to work with an equation rather than a lookup table.

For follower vehicles, a car-follower model has been implemented based on the core NETSIM car-follower equations. Although there are many car-follower models that have been promulgated by various sources, the one in NETSIM was chosen because it is a well-known and accepted model. The basic principle behind NETSIM's car-follower algorithm is the prevention of vehicles colliding or overlapping. As presented in Aycin 1999, the NETSIM equations are reproduced as equations 4-6.

$$a \text{ or } d = F_1 / F_2 \qquad (4)$$
$$F_1 = - L_g + X_L + (V_L^2 / (2d_L)) - X_f - (V_f dt)-(V_f RT)-(V_f^2 / (2d_f)) \qquad (5)$$
$$F_2 = ((1 / 2)dt^2) + (dtRT) + (V_f\, dT / d_f) \qquad (6)$$

where a or d = acceleration or deceleration rate (m/s^2)
F_1, F_2 = intermediate variables
X_L = distance to rear bumper of leader vehicle from a datum (m)

X_f = distance to rear bumper of follower vehicle from a datum (m)
L_g = length of vehicle plus gap (8.8 m)
V_L = speed of leader vehicle (m/s)
d_L = nominal deceleration rate of leader vehicle (3 m/s^2)
V_f = speed of follower vehicle (m/s)
dt = time-step (s)
RT = reaction time (1.5 s)
d_f = nominal deceleration rate of follower vehicle (3 m/s^2)

The derivation of these equations can be found in Aycin 1999 and details concerning the fixed constants can be found in Kim 2004. All of these equations of motion are employed under a discrete modeling framework. That is, each vehicle is moved and updated according to equations 7 and 8 using a 1-second time-step (dt).

$$Vn = Vo + a\,(dt) \quad (7)$$
$$Xn = Xo + Vn\,(dt) \quad (8)$$

where Vn = new vehicle speed (m/s)
Vo = previous vehicle speed (m/s)
Xn = new vehicle position (m)
Xo = previous vehicle position (m)

The modeling of these simulated vehicle movements allow TRAQSIM to simplify user input requirements. For example, since the simulation automatically builds up queues, the user is not required to specify queue links as is required with CAL3QHC. Similarly, the TRAQSIM user does not have the burden of providing the following CAL3QHC data: mixing zone width, clearance lost time, and saturation flow rate.

Modal Emissions

The modal emissions modeling capability in TRAQSIM is essentially based on a lookup table of CMEM outputs. CMEM was chosen for its ability to model second-by-second emission factors. Other models can also provide this capability, but many of them were developed based on data from older fleets and are not readily available for public use. CMEM allowed relatively easy development of speed-acceleration matrices of emission factors. Indeed, the user's guide exemplifies the development of such lookup tables and suggests their use with traffic simulation models such as NETSIM, FRESIM, etc. [Barth 2001]. Further development of TRAQSIM may incorporate the use of EPA's Motor Vehicle Emissions Simulator (MOVES) which can also generate second-by-second emission factors.

The CEM lookup table was developed by running CMEM on a matrix of speed and acceleration combinations. Speed and acceleration represent the key parameters affecting a vehicle's power demand. The outputs from CMEM that were used to form this lookup table are second-by-second CO emission factors in g/s. The speed and acceleration values range from 0 to 80 mph and –6 to 6 mph/s, respectively. The resulting table (or matrix) of emission factors is based on speed, acceleration, and vehicle ID number.

Three sets of these tables were developed to represent the different operating modes: stable and hot/cold transient modes. The first was developed by setting the soak time parameter for each vehicle type in CMEM to zero. Since the soak time is defined as the engine-off period, setting this value to zero in CMEM results in estimation of emission rates from vehicles that are in a stabilized mode [Barth 2001]. The hot transient lookup table was developed by setting the soak time for each vehicle to 10 minutes and the cold transient lookup table was developed by setting the soak times to 1440 minutes (24 hours) as prescribed in the CMEM User's Guide [Barth 2001]. Future improvements to TRAQSIM could involve providing these soak times as user inputs such that TRAQSIM could generate the lookup tables dynamically at the beginning of a model run. This would allow for the possibility of modeling "intermediate" soak times such as 1 or 2 hours.

User-supplied hot, cold, and stabilized percentages are used as a distribution of engine-conditions to randomly assign each vehicle to one of these modes. Therefore, based on this assignment, the appropriate lookup table is used to model each vehicle's emission factors. Since the engine-on period of each vehicle is unknown prior to its arrival at the intersection, a change in mode (i.e., transient to stabilized) cannot be properly modeled. Therefore, all vehicles are assumed to stay in the originally assigned engine conditions. This is a reasonable assumption in part because vehicles generally spend much less than 505 seconds at an intersection. Also, the modeling of constant modes is in keeping with the need to uphold the input percentages. If the modes changed, then the percentages would not be accurately modeled.

In addition to the 26 light-duty CMEM vehicles used in TRAQSIM, scaling factors were employed to model additional vehicle types not covered by CMEM. The scaling factors were derived by comparing typical MOBILE6-computed emission factors for light-duty gas vehicles (LDGV) with 5 other vehicle types. From analyzing example distributions provided in the CMEM User's Guide [Barth 2001], the most popular light-duty gas-powered vehicle appears to be CMEM vehicle 5 (i.e., closest to the MOBILE6 LDGV category). These scaling factors were then used to develop regression fits details of which can be found in Kim 2004. Essentially, the scaling factors for each of the vehicle types represent normalizations by the emission factor for the LDGV vehicle type at the corresponding speed.

Atmospheric Dispersion

Atmospheric dispersion modeling within TRAQSIM is based on the use of Gaussian puffs in a Lagrangian framework. The concentration contribution from a single puff at a receptor location is calculated from Equation 9.

$$c = \frac{\Delta M}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left[-\frac{1}{2}\left(\frac{x_p - x_r}{\sigma_x}\right)^2\right]\exp\left[-\frac{1}{2}\left(\frac{y_p - y_r}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z_p - z_r}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z_p + z_r}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2H_m - z_p - z_r}{\sigma_z}\right)^2\right]\right\} \quad (9)$$

where c = concentration at a receptor (ppm)
ΔM = mass of puff (g)
σ_x, σ_y, σ_z = dispersion parameters representing the standard deviations of a Gaussian distribution in the x, y, and z directions.
x_p, y_p, z_p = x, y, and z-position of puff center in absolute coordinates (m)
x_r, y_r, z_r = x, y, and z-position of a receptor location (m)
H_m = mixing height (m)

The last exponential term in Equation 9 accounts for reflections from the ground and the mixing height. Although multiple reflections can be modeled, it was not deemed necessary since the mixing height in the range of about 1000 m is too far above typical receptor heights to have much of an effect. Also, for similar reasons, penetrations through the mixing height were not modeled. The determination of the dispersion parameters is based on aggregating the different dispersion effects as shown in equations 10-12.

$$\sigma_x = (\sigma_{xt}^2 + \sigma_{xr}^2 + \sigma_{xw}^2)^{1/2} \quad (10)$$
$$\sigma_y = (\sigma_{yt}^2 + \sigma_{yr}^2 + \sigma_{yw}^2)^{1/2} \quad (11)$$
$$\sigma_z = (\sigma_{zt}^2 + \sigma_{zr}^2 + \sigma_{zw}^2)^{1/2} \quad (12)$$

where σ_x, σ_y, σ_z = composite dispersion parameters (m)
σ_{xt}, σ_{yt}, σ_{zt} = x, y, z dispersion parameters from atmospheric turbulence (m)
σ_{xr}, σ_{yr}, σ_{zr} = x, y, z dispersion parameters from atmospheric rise (m)
σ_{xw}, σ_{yw}, σ_{zw} = x, y, z dispersion parameters from vehicle wake effects (m)

The dispersion due to atmospheric turbulence is modeled through the use of the well-known Pasquill-Gifford dispersion parameters [Turner 1994] presented as equations 13 and 14.

$$\sigma_{xt} = \sigma_{yt} = \{1000r\tan[a - b\ln(r)]\}/2.15 \quad (13)$$
$$\sigma_{zt} = cr^d \quad (14)$$

where r = puff cumulative horizontal travel distance (km)
a, b, c, d = coefficients based on stability class

The cumulative travel distance (r) is the total travel distance traveled by the puff in all three dimensions rather than the distance away a source. The contributors to this total distance include the mean wind, vehicle wake effects, and atmospheric rise (i.e., buoyancy). The mean wind is varied with height based on the use of a power law equation [Turner 1994]. Further details on puff movement modeling can be found in Kim 2004. The dispersion due to atmospheric rise is calculated using equation 15.

$$\sigma_{xr} = \sigma_{yr} = \sigma_{zr} = \Delta H/3.5 \quad (15)$$

where ΔH = atmospheric rise height (m)

Atmospheric rise is modeled using Briggs' well known buoyancy flux and gradual rise equations [Briggs 1971, 1972, and 1975]. The determination of the effects of vehicle wakes on dispersion is based on the use of equations developed by Eskridge and others [Eskridge 1979, 1982, and 1983]. Equations 16-24 describe the velocity field experienced by a puff within a vehicle's wake region.

$$u_d = UA(S)^{-3/4}f(N/l(s), Z/l(s)) \quad (16)$$
$$S = s/H \quad (17)$$
$$Z = z/(\gamma AH) \quad (18)$$
$$N = n/(\lambda\gamma Aw_d) \quad (19)$$
$$A = (C_d/(32\pi e^{1/2}\lambda\gamma^3))^{1/4} \quad (20)$$
$$l(s) = \lambda AH(S)^{1/4} \quad (21)$$
$$f(N/l(s), Z/l(s)) = (Y(N/l(s)))(T(Z/l(s))) \quad (22)$$
$$Y(N/l(s)) = C_1Exp(-N^2/(8l^2(s))) \quad (23)$$
$$T(Z/l(s)) = T(\xi) = \sum b_i\xi^{i-1} + b_0, \text{ for } i = 1 \text{ to } 6 \quad (24)$$

where u_d = velocity deficit (m/s)
U = wind speed relative to vehicle (m/s)
A = Strength of the wake
s = distance behind the vehicle along wake centerline (m)
H = height of vehicle (m)
W_d = width of vehicle (m)
z = vertical distance above the wake centerline (m)
n = distance perpendicular to the wake centerline (m)
γ = constant $\approx$ 0.095
λ = constant $\approx$ 1.14
C_d = drag coefficient
ξ = polynomial variable
b_i = curve fit parameter

A velocity deficit value can be calculated for a point within a vehicle's wake by specifying its distance behind the vehicle along the centerline of the wake, the perpendicular distance from the centerline, and the height above the ground. The velocity deficit is essentially a relative velocity (relative to the mean wind) that is parallel to the centerline of the wake. Application of this relative velocity to a puff represents the dragging effect of a vehicle's wake. This dragging movement of a puff contributes to the aforementioned total distance traveled, and thereby contributes to the atmospheric turbulence term (σ_{xt}, σ_{yt}, and σ_{zt}). The direct dispersion due to the vehicle's wake is determined from equations 25-28.

$$u'^2, v'^2, w'^2 = (a_1, a_2, a_3)A^2U^2S^{-1.2}F_c(\chi,\omega) \quad (25)$$
$$\chi = n/(W_ds^{0.4}) \quad (26)$$
$$\omega = z/(Hs^{0.4}) \quad (27)$$
$$F_c(\chi,\omega) = \sum_n\sum_m\psi_{2m,n}\omega^n\chi^{2m}, \text{ for } m = 0 \text{ to } 2 \ \& \ n = 0 \text{ to } 4 \quad (28)$$

where u'^2, v'^2, w'^2 = velocity variances
a_1, a_2, a_3 = constants = 0.048, 0.040, and 0.030, respectively
if $|\chi| \geq 0.55$ or $|\omega| \geq 0.64$ then $F_c = 0$
if $\chi \leq 0.0$ and $\omega > 1.82\chi + 1.15$ then $F_c = 0$
if $\chi > 0.0$ and $\omega > -1.82\chi + 1.15$ then $F_c = 0$
if $Z/l(s) > 8.2$ then $T(Z/l(s)) = 0$
ψ = surface fit parameter

The velocity variances determined from Equation 25 can be correlated to dispersion parameters by using Pasquill's relationships [Pasquill 1971] which Draxler rewrote [Draxler 1976]. See Kim 2005 for details on this relationship.

In an effort to reduce computational burdens on a computer, a puff merging process was implemented. Merging reduces the number of puffs that need to be modeled. The scheme is based on a recommendation made by Ludwig, et al. [Ludwig 1976] who indicated that two puffs whose centers are separated by up to two sigma values could be combined with minimal effects on accuracy. In TRAQSIM, the merging algorithm first determines the 3-dimensional distance between the centers of a pair of puffs. This distance is then compared to the sum of the average sigma values of each of the puffs. An average sigma value for a puff refers to an average of the three sigma values associated with dispersion in 3-dimensions (i.e., x, y, and z). When two puffs are merged, the resulting single puff is created midway between the two puffs and contains attributes that are either an average or the sum of the two puffs. For example, the sigma values are averages while the mass of pollutant is a sum.

VALIDATION

For the initial validation work, two studies were conducted. The first involved comparisons against CAL3QHC to examine model behavior. Second, comparisons against high-quality measured field data were conducted.

For the relative comparisons against CAL3QHC, a simple line source was used to exemplify some of the fundamental differences between the two models. Since all of the input data for each model were identical (or as close as possible), the comparisons show differences between each model's underlying data and methods. As shown in Figure 1, the scenario involved a single roadway (link) with one signal and 15 receptors.

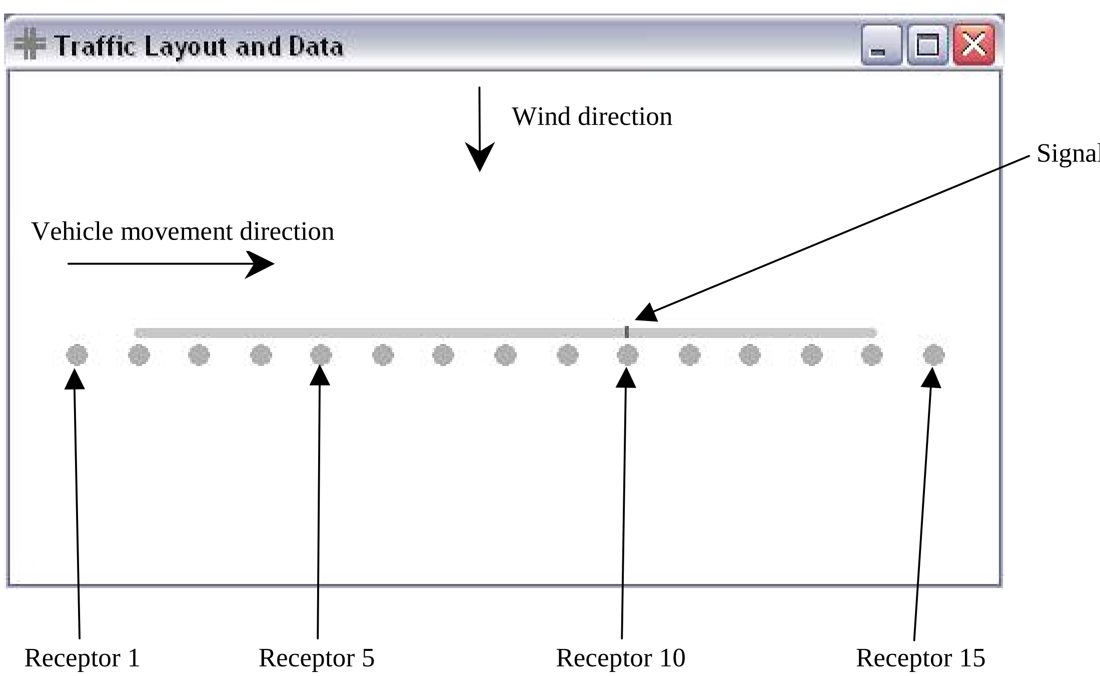

Figure 1. Single Roadway Scenario

The associated scenario data are shown below:

- Vehicles per hour = 400
- Wind speed = 2 m/s
- Wind direction = 0 degrees
- Stability class = D
- Vehicle cruise speed = 35 mph
- Vehicle types = only light-duty vehicles
- Signal Timing: Green = 20 sec, Yellow = 2 sec, and Red = 40 sec

The average emission factors (i.e., of cruise and idle) for CAL3QHC were derived from TRAQSIM at the appropriate speeds. This allowed a focused comparison of just the dispersion methods within in each model. The modeled concentrations are shown in Figure 2.

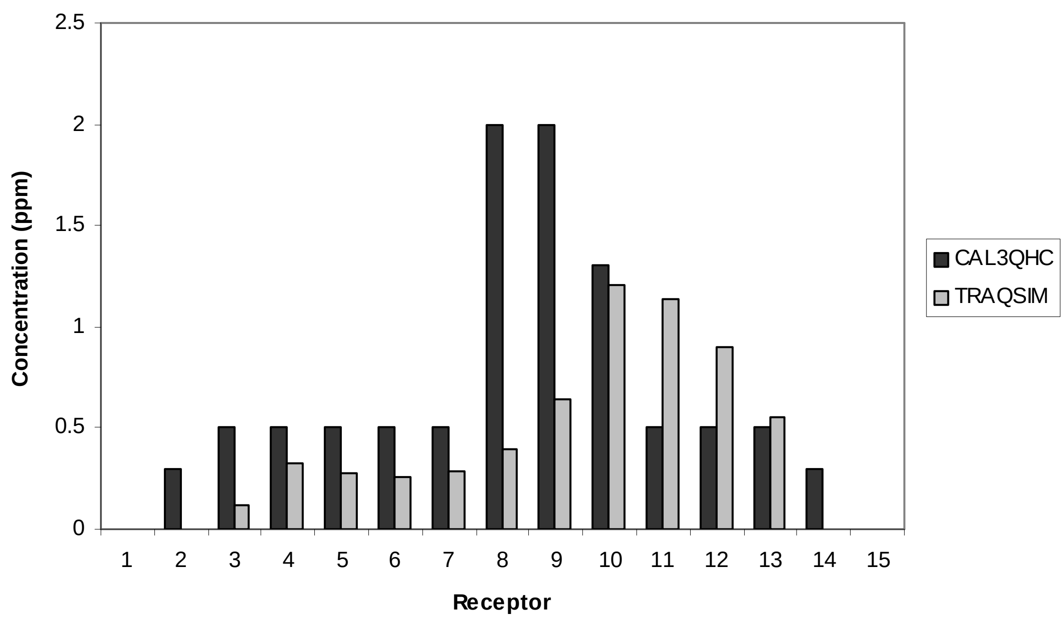

Figure 2. Modeled Results of Simple Straight Roadway Scenario

The higher concentrations occur toward the middle of the link and generally decrease towards the ends. This is intuitive since the wind direction (0 degrees) is directly downward and the receptors near the middle experience a greater contribution of pollutants. It should be noted that some of the concentrations (e.g., for receptors 1 and 14) are too small to be "seen" in Figure 2. The higher concentrations from the two models are not coincidental. CAL3QHC models highest concentrations at receptors 8-10 which are closest to the queue section of the link (just behind the signal). In contrast, TRAQSIM models highest concentrations at receptors 10-12 which are closer to the acceleration section of the link. The results from TRAQSIM appear to be more intuitive since time-based emission rates from acceleration are generally greater than idle partly due to fuel enrichment during acceleration. Also, vehicle wakes also likely dragged some of the pollutants toward receptors 10-12. These results appear to indicate that TRAQSIM's use of puffs in a traffic simulation environment provides more realistic modeling of the physical phenomena occurring at intersections. TRAQSIM's results appear to make more intuitive sense.

In addition to the relative comparisons against CAL3QHC, a major validation exercise was conducted using high-quality field data. The work actually involved comparing the modeled results of both CAL3QHC and TRAQSIM to the measured data.

The data was obtained from a major field collection effort that was conducted in the 1993-1995 period as part of an NCHRP-sponsored project [Carr 1996]. The data were collected from intersections at Tucson, Arizona and Denver, Colorado, and they included all of the meteorological and traffic data in 15-minute averages (intermediate values developed from the truly raw data which were collected in resolutions of seconds and minutes). However, only the data from the Denver site was considered for this validation exercise in part because it was generally considered to be more reliable since the Denver site was the second site to be included in the measurements. Since the Denver data was too voluminous for all of it to be used, only a few hours worth of data were processed; but these few hours still resulted in over 260 data points.

In general, the processing involved determining 1-hour averages or totals from the 15-minute values. Much of the data, especially the traffic data, had already been processed by the source and provided as representative data. The database included the following types of information:

- Meteorology
- Geometric layout of roadways
- Receptor locations
- CO concentrations
- Traffic volumes
- Traffic turning volumes
- Vehicle speeds
- Signal timings
- MOBILE5 input file

For the meteorological data, 1-hour averages were developed for CAL3QHC but 15- minute values were used in TRAQSIM. TRAQSIM allows multiple time-varying meteorological data to be used. Therefore, 4 sets of wind speed, wind direction, and temperature as well as their measurement heights were used in TRAQSIM. An overall stability class was determined from using average values of wind speed, standard deviation of the change in wind direction, and their associated heights for each hour modeled. Specifically, EPA's definition of stability classes were followed [EPA 1986].

The geometric positions of roadways (links) were based on a representative overhead drawing of the intersection provided as part of the data that was approximately to scale. All links were assumed to have zero height (i.e., z = 0 m). A total of 60 links were modeled.

The processing of the CO concentrations was straightforward. First, the 15-minute values were averaged into 1-hour concentrations. Then background concentrations were determined by choosing an appropriate upwind receptor. This agrees with the usual definition for verification/validation studies and was considered more accurate than trying to determine a general nominal background value for the Denver area [Cooper 1987].

The traffic volumes were totals for each direction (i.e., rather than each lane) and were specific to each 15-minute period in each day. In contrast, the turning volumes were just representative values for 15-minute periods gathered over two days. Therefore, the turning volumes were used to derive representative fractions of turns that were applied to the approach traffic volumes.

Similar to the turning movement data, the speed data were also representative values measured over three days and categorized into AM and PM periods and direction (e.g., westbound, southbound, etc.). The speed samples for each of these categories were plotted and two peaks were identified in each of the distributions (i.e., a bimodal distribution). The higher peak was used to identify the cruise speed.

Signal timing data were also just representative values specific to only the AM and PM periods of the day. A total of 17 signals (one signal per link) were created in order to properly model the interrupted traffic flows. These signals were grouped into 8 categories corresponding to the through and turning traffic.

The MOBILE5 input file was used as the basis for the development of the MOBILE6.2 input file. Guidelines in the MOBILE6.2 User's Guide [EPA 2002] were followed in converting the MOBILE5 file. In addition to the MOBILE6.2 input data, the MOBILE5 VMT fractions were also used to determine the VMT fractions of CMEM vehicle types. To do this, the age distributions from the MOBILE5 file were used in conjunction with the guidelines in the CMEM User's Guide [Barth 2001].

The results of the modeled versus measured comparisons are presented in Table 1.

Table 1. Statistical Parameters from comparing Modeled versus Measured Concentrations

Stability Conditions	Statistical Parameter[a]	CAL3QHC	TRAQSIM
All	Number of Data Points	264	264
	Overall Error	2.180	4.084
	Bias	0.393	2.629
	-/+ 95% Confidence Interval	0.260	0.379
	Random Error	1.587	1.726
	Correlation Coefficient, r	0.849	0.778
	Coefficient of Determination, R^2	0.721	0.605
	Slope	1.265	1.409
	Y-Intercept	-0.429	1.357
Unstable/Neutral (A-D)	Number of Data Points	144	144
	Overall Error	1.287	2.998
	Bias	-0.244	1.942
	-/+ 95% Confidence Interval	0.209	0.378
	Random Error	1.309	1.310
	Correlation Coefficient, r	0.553	0.497
	Coefficient of Determination, R^2	0.305	0.247
	Slope	0.416	0.886
	Y-Intercept	0.886	2.144
Stable (E-F)[b]	Number of Data Points	120	120
	Overall Error	2.911	5.089
	Bias	1.157	3.452
	-/+ 95% Confidence Interval	0.485	0.679
	Random Error	1.588	1.854
	Correlation Coefficient, r	0.850	0.768
	Coefficient of Determination, R^2	0.722	0.590
	Slope	1.430	1.529
	Y-Intercept	-0.869	0.961

[a] Definitions of statistical parameters are provided in Appendix E.
[b] All data were based on F stability classes (i.e., there were no E stability classes).

All of the plots and statistical parameters were generated using a commercially-available software package, STATISTICA [StatSoft 2001]. The overall and stable stability class comparisons show relatively "good" agreement with measured data by both models. CAL3QHC and TRAQSIM show R^2 values of 0.721 and 0.605 overall and R^2 values of 0.722 and 0.590 for the stable cases, respectively. Although the unstable-neutral conditions show poor agreement (R^2 values of 0.305 and 0.247), it was expected due to the difficulties of modeling unstable-neutral conditions. These conditions are more difficult to model accurately because the dispersion modeling components (e.g., atmospheric rise) have greater uncertainties. And since stable conditions are more important in terms of conservative modeling, the focus of these comparisons should be on the stable (and overall) conditions. In general, the results appear to show that TRAQSIM is more conservative than CAL3QHC.

All of the comparison plots and the statistical parameters appear to show CAL3QHC outperforming TRAQSIM. However, since the statistical parameters are relatively close in many cases, it may be inappropriate to conclude that CAL3QHC is a better model than TRAQSIM. For example, the Random Error statistics are relatively close (especially for the unstable/neutral category) and it would be difficult to judge one model over the other. For these types of modeled versus measured comparisons, the Random Error statistic may be one of the better gauges of performance. In the future, further analyses at other locations with many more data points should be conducted before a definitive judgment can be made.

A deeper inspection of some of the results indicate that while overall CAL3QHC may appear to generally perform better, some of the TRAQSIM results are more attractive. For example, CAL3QHC shows negative y-intercepts for the all and stable categories while TRAQSIM's y-intercepts are positive. Also, the negative bias that CAL3QHC exhibits for the unstable-neutral category is unattractive as it may indicate a trend toward underprediction. In contrast, the bias for TRAQSIM is positive. In general, it is preferable for models of this type to over-predict rather than under-predict (i.e., especially in a regulatory-type setting). In addition, when comparing on an individual scenario basis, the results were mixed. Table 2 shows R^2 values for each of the 11 scenarios.

Table 2. R^2 values for each Scenario

Scenario Number	CAL3QHC R^2	TRAQSIM R^2
1	0.479	0.357
2	0.285	0.639
3	0.391	0.398
4	0.830	0.382
5	0.618	0.132
6	0.215	0.250
7	0.598	0.573
8	0.669	0.561
9	0.345	0.630
10	0.614	0.607
11	0.365	0.458

Note: Highlighted values indicate better aggrement with measured data. Each scenario is composed of 24 data points.

As indicated in Table 2, the results on a scenario-by-scenario basis was about evenly split with CAL3QHC performing better in 6 scenarios while TRAQSIM performed better in 5 scenarios. Although other statistical parameters could be added to this table for a more complete comparison, these R^2 values illustrate the difficulty of making definitive conclusions about one model performing better than the other. As previously indicated, additional scenarios with more data points will need to be modeled.

It also needs to be mentioned that the performance of the two models could very well be due to the emission factor data from MOBILE and CMEM. Since the Gaussian dispersion equations show emissions as being directly proportional to concentrations, the accuracy of the CMEM data could be a major reason why TRAQSIM appears to under-perform CAL3QHC in certain scenarios. Although CMEM's second-by-second emissions modeling is methodically more correct for use in TRAQSIM, CMEM does not take into account atmospheric conditions (e.g., humidity, pressure, etc.), vehicle ages, inspection and maintenance programs, fuel characteristics, etc. which are included in MOBILE. Future validation assessments could be conducted between MOBILE and CMEM emission factors to determine their effects on concentrations and on model performance parameters such as R^2. Future improvements to TRAQSIM will include the replacement of CMEM with EPA's successor to the MOBILE-series models, the Motor Vehicle Emission Simulator (MOVES), which can generate second-by-second emission factors.

A key component in modeling the emission factors in both MOBILE and CMEM were the representative speed data. Since the original data had already been processed into generic AM and PM categories, they could have introduced a noticeable error into the emission factors. A quick sensitivity check for an average speed of 35 mph with a 5 mph error shows that the resulting emission factor could have an error of about 3% for a LDGV. Other vehicle types such a HDGV could see errors of about 15%. Similarly, noticeable errors were also likely introduced through the use of representative (non-specific) turning movements, and signal timings. As these datasets were not specific to each modeled scenario, they could have caused additional errors, especially since several receptors were relatively close to turning lanes. Although the same traffic data were used with both models (TRAQSIM and CAL3QHC), the magnitude of the errors could have been different between them.

CONCLUSIONS

The development of TRAQSIM was an experiment to see if a more realistic and flexible model than CAL3QHC could be developed through the use of a simulation approach. The use of traffic simulation and puff dispersion methodologies allowed the use of the model to be relatively straightforward. That is, the input data requirements and scenario setup are more intuitive for the user than CAL3QHC. This is due to the fact that CAL3QHC models physical phenomena through macroscopic methods whereas TRAQSIM models physical phenomena at a more fundamental (or detailed) level. For example, details such as queue link positions and saturation flow rates do not need to be specified in TRAQSIM as they are in CAL3QHC. These types of input data burdens do not exist in TRAQSIM.

As part of the initial validation work, a relative comparison against CAL3QHC showed that the modal emissions modeling and puff movement due to vehicle wake effects in TRAQSIM appear to produce more intuitive results as exemplified through a simple line source test. However the validation comparisons against field data appear to favor CAL3QHC with R^2 values of 0.721 and 0.605 for CAL3QHC and TRAQSIM, respectively, on an overall basis. One of the reasons for these results may have been due to the emission factors from CMEM which may not have been as accurate as those from MOBILE since CMEM does not take into account such effects as atmospheric conditions, vehicle ages, fuel characteristics, etc. Also, the non-specificity of the speed and turning-movement data could have caused some noticeable errors as well.

Although the statistical parameters appear to show CAL3QHC outperforming TRAQSIM, certain parameters (e.g., y-intercept and bias) were more attractive for TRAQSIM. For example, the positive y-intercepts and positive biases were more attractive since it is preferable to have a model over-predict than under-predict, especially in a regulatory-type setting. Also, on a scenario-by-scenario basis, the results were mixed such that CAL3QHC showed higher R^2 values for 6 scenarios while TRAQSIM showed higher R^2 values for 5 scenarios. Therefore, additional comparisons with larger datasets at other locations will need to be conducted to arrive at a more definitive conclusion regarding model performance. Also, while CAL3QHC is a mature model that has been developed over many years, TRAQSIM is new and has much more potential for improvement. The physical parameters used in TRAQSIM allow it to be more directly (more logically) improved than the approximations used in CAL3QHC. It is anticipated that further model improvements including the replacement of CMEM with EPA's MOVES will make TRAQSIM a more accurate and useful model.

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