Predicting Air Quality Near Roadways through the Application of a Gaussian Puff Model to Moving Sources

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ABSTRACT

The Environmental Protection Agency (EPA) currently recommends the use of CALINE3 or CAL3QHC for modeling the dispersion of carbon monoxide (CO) near roadways. These models treat vehicles as part of a line source such that the emissions are homogeneously spread out over the entire line. And since the models use Gaussian plume equations, the results are inherently steady-state values.

This paper describes a new simulation model entitled, TRaffic Air Quality SImulation Model (TRAQSIM), developed at the University of Central Florida. The basic concept in the model is that each vehicle is considered a discrete moving point source rather than as part of an overall line or area source. The model simulates traffic movement and keeps track of the properties of each vehicle as it moves through a traffic scenario. During each time-step, vehicles are moved and assigned mode-varying emission factors. The dispersion in the atmosphere is accomplished through the use of a Gaussian puff algorithm. Dispersion parameters (σs) are determined from Pasquill stability classes and combined with dispersion parameters corresponding to thermal buoyancy and vehicle wake effects. Puff merging has also been implemented to reduce computer processing time.

INTRODUCTION

The Environmental Protection Agency (EPA) currently recommends the use of CALINE3 or CAL3QHC for modeling the dispersion of Carbon Monoxide (CO) near roadways. These models distribute vehicle emissions and traffic volumes along roadways which are modeled as line sources. This approach is not realistic because only constant speed (not modal) emission factors are applied to the line sources. Also, since the models handle atmospheric dispersion through the use of steady-state Gaussian equations, time-varying input and output information cannot be applied.

This paper describes a new roadway and intersection air quality model developed at the University of Central Florida (UCF) entitled, TRaffic Air Quality SImulation Model (TRAQSIM). The model takes a simulation approach such that each vehicle is treated as a discrete moving point source. Emissions from these moving sources are mode-specific since modal multipliers are used to convert constant speed emission factors to modal emission factors. The development of the modal multiplier regression equations from the cooperative industry/government emissions database collected in 1993-1994 is described elsewhere (1). Atmospheric dispersion modeling is accomplished through the use of Gaussian puff equations in order to provide transient concentrations. It is believed that these theories provide a greater degree of accuracy and versatility to the overall model than the current regulatory models.

COMPARABLE MODELS

Of the two EPA recommended models, CAL3QHC is more appropriate than CALINE3 in comparing to TRAQSIM because unlike CALINE3, CAL3QHC can model interrupted flow (intersections). CAL3QHC takes a macroscale approach in determining queue lengths by using established methods from literature such as the Highway Capacity Manual (2). Acceleration and deceleration modes are approximated by using queue links. Therefore, vehicle modes are not handled in a realistic manner. The cruise mode is handled identical to constant speed travel along free-flow links, but the idle mode is approximated by converting queue lengths into equivalent free-flow line sources. Acceleration and deceleration effects are approximated by the use of excess emissions which are derived by converting queue links to equivalent free-flow links. All of the emissions are used in Gaussian plume equations for line sources. CAL3QHC essentially uses the CALINE3 model for atmospheric dispersion. Due to the steady-state nature of the equations used, time-varying data (e.g. meteorological) cannot be used during a model run. Although wind angles can be varied and additional runs can be made for different conditions, the results would still be steady-state concentrations. A well-known shortcoming of CAL3QHC and most other air quality roadway models is that dispersion in the near field due to vehicle wake effects and thermal turbulence is difficult or impossible to accurately model. This is because CALINE3 uses a mixing zone concept to account for the initial dispersion directly over a roadway. The mixing zone is described by setting an initial σ_z three meters downwind of the nearest lane.

TEXIN2-4 is similar in scope to CAL3QHC in that it can model interrupted flow and also employs the same equations used in CALINE3 to model dispersion. However, the excess emissions arising from queues is handled differently. TEXIN2-4 uses Critical Movement Analysis (CMA) to determine a volume to capacity ratio (v/c) that leads to the determination of the queue length. This queue length is then used along with derived emission factors for vehicles slowing, stopping, and idling to determine the total excess emission factor (3).

The CALINE4 model is essentially an expansion of CALINE3. Unlike its predecessor, CALINE4 can be used to to model intersections. Queue lengths are determined by using a vehicle spacing distance of seven meters and modal activity input data. Modal emission factors are determined from exponential functions obtained from regression analyses involving modal multipliers and the product of speed and acceleration. These factors are used to determine cumulative modal emission profiles for each link. For use in dispersion modeling, the average distance rate emission factor (e.g. g/mile) for a link is obtained by dividing the difference between cumulative emissions at the link ends by the length of the link. Similar to CALINE3, CALINE4 also incorporates a mixing zone concept to account for the initial dispersion directly over a roadway. But CALINE4 expands upon this methodology by incorporating an upward heat flux algorithm that modifies the σ_z values (4).

FLINT is another intersection air quality model that was developed at the University of Central Florida. It uses macroscale traffic theory to determine queue lengths and lengths of the acceleration/deceleration zones. Modal emission factors are determined by applying fixed multipliers to constant speed emission factors. The method FLINT uses to model roadways is different than the aforementioned models in that the roadways are treated as area sources and not as line sources. Dispersion is accomplished through the use of the area source algorithm within the PAL2 model. However, the σ values in PAL2 were replaced with the ones in CALINE3 (5).

MODEL DEVELOPMENT THEORY

Vehicle Emissions

TRAQSIM currently requires constant speed emission factors determined from MOBILE5a. These factors are converted to modal emission factors by the use of modal multipliers. The development of the modal multiplier regression equations is presented in another paper (1). The equations relate modal multipliers (dependent variable) to the product of vehicle speed and acceleration (independent variable). Emissions are categorized in terms of vehicle type (cars, light-trucks, and heavy light-trucks) and engine condition (cold transient, hot transient, and stabilized). The condition of the engine is assumed to be constant for each vehicle as it moves through a traffic scenario. This is considered reasonable since travel times through an intersection are relatively short and the condition of the engine is unknown prior to a vehicle's emergence into the intersection being modeled.

Atmospheric Dispersion

Dispersion in the atmosphere is modeled through the use of a Gaussian puff algorithm. The basic equation describing the concentration at a point in space due to a single puff of pollutant is presented as equation 1.

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

where c = concentration (g/m^3)
Q = emission factor (g/s)
Δt = time interval between puff release (s)
x_p, y_p, z_p = center of puff (m, m, m)
x_r, y_r, z_r = receptor location (m, m, m)
H_m = height of mixing zone (m)
σ_x = standard deviation of puff in the x-direction (m)
σ_y = standard deviation of puff in the y-direction (m)
σ_z = standard deviation of puff in the vertical (z) direction (m)

The last two exponential terms in equation 1 represent reflections from the ground and the top of the mixing zone, respectively. Due to the conservative nature of CO, no deposition or decay is taken into account. Although wind speed is not shown in the equation, it can be incorporated into the puff location terms because a puff will be advected by the mean wind. In addition to the wind, a puff's movement (or position) will be affected by atmospheric rise and vehicle wake effects. These different components also cause dispersion the magnitudes of which can be combined as shown in equations 2-4.

$$\sigma_x^2 = \sigma_{ht}^2 + \sigma_{hr}^2 + \sigma_{xw}^2 \qquad (2)$$

$$\sigma_y^2 = \sigma_{ht}^2 + \sigma_{hr}^2 + \sigma_{yw}^2 \qquad (3)$$

$$\sigma_z^2 = \sigma_{zt}^2 + \sigma_{zr}^2 + \sigma_{zw}^2 \qquad (4)$$

where σ_x = x-composite horizontal dispersion parameter (m)
σ_y = y-composite horizontal dispersion parameter (m)
σ_{ht} = horizontal dispersion parameter corresponding to atm. turbulence (m)
σ_{hr} = horizontal dispersion parameter corresponding to atm. rise (m)

σ_{xw} = x-horizontal dispersion parameter corresponding to vehicle wake effects (m)
σ_{yw} = y-horizontal dispersion parameter corresponding to vehicle wake effects (m)
σ_z = composite vertical dispersion parameter (m)
σ_{zt} = vertical dispersion parameter corresponding to atmospheric turbulence (m)
σ_{zr} = vertical dispersion parameter corresponding to atmospheric rise (m)
σ_{zw} = vertical dispersion parameter corresponding to vehicle wake effects (m)

Dispersion parameters corresponding to atmospheric turbulence are calculated from equations 5 and 6 which are based on parameters for quasi-instantaneous sources that Turner developed from Slade (6).

$$\sigma_{ht} = ar^b \quad (5)$$

$$\sigma_{zt} = cr^d \quad (6)$$

where r = puff travel distance (m)
a, b, c, d = coefficients based on stability class (Table 1)

The parameters for these equations are shown in Table 1. This method of determining dispersion parameters is similar to those used by current regulatory line source models. Although theoretically simple, it is advantageous over other methods when considering computation time. The travel distance (r) in equations 5 and 6 is not necessarily the linear distance from a current puff position to its original (release) position. Rather, r is the total travel distance along the entire pathway from the puffs original position to its current position in time.

Atmospheric rise is modeled by the use of the solutions presented by Hurley and Physick (7). Their equations for vertical rise and corresponding dispersion parameters are reproduced as equations 7-11.

$$z_r = 1.6[(F_o t^2)/u_h]^{1/3} \quad (7)$$

$$F_o = g w_s r_s^2[1-(T_a/T_s)] \quad (8)$$

$$R = \beta z_r \quad (9)$$

$$\sigma_{hr} = R \quad (10)$$

$$\sigma_{zr} = R/2 \quad (11)$$

where z_r = rise distance (current – original) (m)
F_o = buoyancy factor (m^4/s^3)
t = time (s)
u_h = ambient horizontal wind speed (m/s)
g = gravitational constant = 9.81 m/s^2
w_s = exit velocity (m/s)

r_s = exit radius (m)
T_a = ambient temperature (K)
T_s = exit temperature (K)
R = horizontal radius of puff = horizontal dispersion parameter (m)
β = constant ≈ 0.6

Equation 7 ignores momentum effects which is reasonable since buoyancy is usually considered to be the dominant factor in atmospheric rise (8). In addition, emissions from vehicles are usually horizontal and therefore, do no contribute to vertical momentum. Although these equations were derived for plumes, they are justified for use with puffs since puffs can be used to model plumes.

Of all the movement and dispersion factors affecting puffs, vehicle wake effects are probably the most complicated. A vehicle's wake can affect nearby puffs through aerodynamic drag and turbulent dispersion. Drag forces can carry emissions behind a vehicle resulting in a "channel" of pollutants along the roadway. Although this can affect pollutant concentrations at receptor locations, aerodynamic drag (also called wake passing effect) is inherently non-dispersive. Its effect on dispersion occurs indirectly through its contribution to the mean velocity. The wake can be modeled as a self-preserving region generally behind a moving vehicle where the velocity of a point in the region decreases with distance away from the vehicle in three dimensions. The vehicle wake theory was originally developed by Eskridge and Hunt and modified by Eskridge and Thompson, and Eskridge and Rao (9, 10, and 11). Their equations for the velocity field and the turbulent energy in the wake are reproduced as equations 12-24.

$$u_d = UA(S)^{-3/4} f(N/l(s), Z/l(s)) \quad (12)$$

$$S = s/H \quad (13)$$

$$Z = z/(\gamma AH) \quad (14)$$

$$N = n/(\lambda\gamma A w_d) \quad (15)$$

$$A = [Cd/(32\pi e^{1/2}\lambda\gamma^3)]^{1/4} \quad (16)$$

$$l(s) = \lambda AH(S)^{1/4} \quad (17)$$

$$f(N/l(s), Z/l(s)) = [Y(N/l(s))][T(Z/l(s))] \quad (18)$$

$$Y(N/l(s)) = C_1 \mathrm{Exp}[-N^2/(8l^2(s))] \quad (19)$$

$$T(Z/l(s)) = T(\xi) = \sum b_i \xi^{i-1} + b_0, \text{ for } i = 1 \text{ to } 6 \quad (20)$$

$$(u'^2, v'^2, w'^2) = (a_1, a_2, a_3)A^2U^2S^{-1.2}F_c(\chi,\omega) \quad (21)$$

$$\chi = n/(W_d s^{0.4}) \quad (22)$$

$$\omega = z/(Hs^{0.4}) \quad (23)$$

$$F_c(\chi,\omega) = \sum_n\sum_m \psi_{2m,n}\omega^n\chi^{2m}, \text{ for m = 0 to 2 \& n = 0 to 4} \quad (24)$$

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 the 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 ≈ 0.095
λ = constant ≈ 1.14
C_d = drag coefficient
u'^2, v'^2, w'^2 = velocity variances
a_1, a_2, a_3 = constants = 0.048, 0.040, 0.030

The velocity variances determined from equation 21 can be correlated to dispersion parameters by using equation 25 which is derived from Taylor's formula (12).

$$(\sigma_{xw}^2, \sigma_{yw}^2, \sigma_{zw}^2) = (u'^2, v'^2, w'^2)t^2 \quad (25)$$

Equation 25 assumes that the travel time is much smaller than the Lagrangian time scale which is typically on the order of 100 to 200 seconds (13). Since TRAQSIM uses a much smaller time step (one second) during simulation, the use of equation 25 appears to be justified.

The coefficients for equations 20 and 24 are shown in Table 2. The wake equations are based on a coordinate system relative to the moving vehicle. This is evident in Figure 1 which shows a simplified view of a wake that has been shifted from the centerline of a roadway due to the mean wind. Using this coordinate system, the velocity deficit is defined as the difference between the velocity of the ambient air moving past the vehicle and the velocity of the air in the wake region. Therefore, the air immediately behind the vehicle would have the highest velocity deficit. Depending on the coordinate system used, the mean wind would affect the velocity deficit and should be incorporated accordingly.

Traffic Simulation

The movement of vehicles is handled through a simulation module originally developed for the Community Noise Model (CNM) developed at UCF under sponsorship by the American Automobile Manufacturers Association (AAMA) (14). The code creates, moves, and eliminates vehicles according to the requirements set by the input data (e.g. simulation time, roadway geometry, traffic volume, etc.). Random number generators are implemented to affect vehicle creation time and their initial deployment position on a roadway. This allows the simulation to occur in a stochastic environment where each simulation run will likely be unique even though consecutive runs may use the same input data. However, this uniqueness only applies to the dynamics during the simulation. Experiences from running the CNM model indicate that the differences between concentrations determined under non-extreme conditions (i.e. reasonable simulation time and traffic volumes) for identical input data will likely be trivial.

The traffic simulation module includes several algorithms including traffic follower, start-up loss time, acceleration rates, deceleration rates, signal timing, etc. Most of the values for the parameters used in these modules were taken from literature including those from the Institute of Transportation Engineers (15).

MODEL STRUCTURE

The basic simulation scheme for the overall model is presented in Figure 2. The traffic simulation and modal emission factor modules are condensed for simplicity. As previously mentioned, these modules have been discussed elsewhere and will not be covered in detail here. The simulation begins with an increment in time followed by traffic movement and the determination of mode-specific emission factors. For newly created puffs, initial dispersion parameters (σs) are set based on the size of the exhaust outlet (i.e. tailpipe radius). Meteorological data is read during each time step because the program allows more than one record to be used during a simulation. This data affects all three subroutines (atmospheric turbulence, atmospheric rise, and vehicle wake effects) that control the movement and dispersion of puffs. Of these three, the effects caused by vehicle wakes is the most complex due to the geometry of the vehicle and wake. Since the program has to cycle through each vehicle for each existing puff, wake effects are computationally intensive. Once all of these effects are determined, new dispersion parameters are calculated. This must be done at each time step because some of the dispersion parameters (e.g. from wake effects) must be cumulatively determined. The puffs are then moved horizontally according to the mean wind and vehicle wakes, and vertically according to atmospheric rise effects.

Puff merging is done mainly to reduce computation time. In a merging process, two puffs are replaced by a single puff containing the sum of the masses of the two puffs and average values for all other parameters (σ values). Ludwig et al. suggest the merging of two puffs when the distance between their centers is less than the sum of two σ values (averages from each puff) (16).

Another option to reduce computation time is puff purging which basically refers to the deletion of a puff. When a puff has moved far enough from a receptor location, its contribution to the concentration measured at that receptor may be low enough such that the puff can be effectively purged from further analysis. This may appear to be a simple process requiring only a decision to be made on the cutoff point when a puff will be purged. But since vehicle wakes and changes in the wind field may drag the puff back into the “relevance zone,” purging becomes more complicated. Therefore, purging has not been implemented in the model and will not be used until a reasonable methodology based on sensitivity studies is developed.

In addition to puff merging, Ludwig et al. also discusses the lag (distance and time) between each puff release (16). The use of a distance lag instead of one based on time may be more appropriate because the latter option could be adversely affected by the strength of the mean wind, vehicle wake, and buoyant forces. A fixed time lag may result in an excessive amount of puffs being generated causing stiff processing requirements. And at high wind speeds, not enough puffs would be generated for a fixed time lag such that accuracy would be compromised. Therefore, a constant distance lag would appear to be more appropriate. However, the aforementioned scenarios are based on stationary sources with a constant wind field. For the modeling scenarios in TRAQSIM, any advantages of using constant distance lags for the puffs during their release would eventually be negated by the disruptive effects of vehicle wakes and a changing wind field (e.g. if more than one meteorological record is used). Therefore, a constant time lag of one second is used as the time step during simulation. This approach has the advantage of being computationally simpler and reasonable with respect to a puff being generated each second. But it will eventually need to be validated through a sensitivity analysis.

SOFTWARE DESCRIPTION

The entire software was written in Microsoft Visual BASIC 6.0 for the Windows (95, 98 and 2000) environment. The Visual BASIC compiler may not produce executables that are as optimized as those generated by a C^{++} compiler, but the BASIC programming language clearly has the advantage of clarity and simplicity due to its English-like commands. This is true when comparing the BASIC language to any other language as well. Therefore, the BASIC code is easier to learn and arguably, easier to debug. This provides other novice programmers wishing to modify the program with a shorter comprehension time. These advantages may ultimately outweigh any gains in speed afforded by a more optimized code. The actual losses of speed due to using Visual BASIC instead of a more efficient language remains to be seen, and will not be known unless the code is reproduced using a different language. However, the possibility exists that certain parts of the code could be rewritten in a more efficient language and compiled as a dynamic link library (DLL) which could be used by the main Visual BASIC program as a subroutine.

Due to the Visual BASIC development environment, the model incorporates a user-friendly graphical interface. The design of traffic layouts is accomplished on a cartesian coordinate system and most of the design can be accomplished graphically with minimal keyboard input of coordinates. The graphical nature of the program, especially with the traffic layout editor, simplifies the modeling process and will likely reduce user input errors.

Once all of the input data is entered into the model, the simulation window can be opened to start a run. Once a simulation is started, the traffic layout is reproduced on screen and the traffic animation is shown during the simulation. This allows for a visual check of the modeled scenario. At the end of the simulation, CO concentrations can be obtained for each of the receptor locations from an output window.

TEST RUNS AND VALIDATION

Due to the simulation nature of the model, run time is significantly longer than steady-state models such as CAL3QHC. For example, on a Pentium II 300 megahertz computer with 96 megabytes of ram, the run time for a one hour simulation involving a 400 feet, one-lane roadway with a traffic volume of 300 vehicles per hour came out to be a little over two hours. The run time increases dramatically when the number of traffic elements (e.g. roadways, traffic signals, vehicles etc.) increases. A one hour simulation involving an intersection with 8 major roadway links and 12 minor links (e.g. for turning movements) with about 700 to 800 total vehicles per hour on each of four approach links took approximately 74 hours (over three days). Since run times vary with traffic layout and the computer system used, no average values can be provided. Trial runs with traffic animation features turned off have been previously conducted on the CNM model and results indicate that the animation doesn't make a significant difference in the overall run time. As a result, the animation feature is currently being kept as an integral feature (not optional) in TRAQSIM. TRAQSIM's code is also being modified on an on-going basis in an effort to optimize it, and therefore, the aforementioned run times are likely to be reduced.

Since the validation of any new model is a requirement for its usage, a few preliminary simulations have been conducted using some of the data from the Melrose Park and College Station databases (5). The initial results appear to indicate good correlation with actual CO readings. However several assumptions had to be made with respect to the meteorological and emissions data due to the differences in the models. A more comprehensive validation involving these databases is planned in the near future. It is also hoped that the data collected by Systems Applications International (SAI) under contract to the National Cooperative Highway Research Program (NCHRP) will be made available so that TRAQSIM can be validated with more recent data (17).

CONCLUSION

Taking a simulation approach to modeling air quality near roadways may not be new, but the incorporation of modal emission factors, atmospheric rise, and vehicle wake effects in a single program that uses Gaussian puff dispersion algorithms is unique. The basic advantages that TRAQSIM has over the existing models stem from the simulation approach which is more versatile and realistic than the steady-state algorithms in such models as CAL3QHC. The use of modal multipliers and vehicle wake effects is also more realistic than using equivalent queue lengths and the mixing zone concept, respectively. Although TRAQSIM's current run times on a PC are extremely long (especially for full intersection analysis), code-optimization efforts will likely improve run time in the near future.

RECOMMENDATIONS

There are several recommendations that can be made concerning the new model:

1. The model is being made freely available from the authors to allow a wider range of testing and validation. Validation with data from SAI needs to be done.
2. Sensitivity analyses involving the individual modules (e.g. atmospheric rise, wake effects, etc.) need to be conducted.
3. The use of DLLs created with a more efficient compiler (such as the one used with Visual C^{++}) should be investigated.
4. Incorporating the output from a more complex traffic model (such as CORSIM) should be investigated.
5. TRAQSIM can be merged with the CNM noise model. This would be ideal since the composite model would be able to predict both air and noise quality using the same input data.

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Table 1
Power Function Coefficients for Dispersion Parameter Equations

Stability Class	a	b	c	d
A	0.18	0.92	0.72	0.76
B	0.14	0.92	0.53	0.73

C	0.1	0.92	0.34	0.72
D	0.06	0.92	0.15	0.70
E	0.045	0.91	0.12	0.67
F	0.03	0.90	0.08	0.64
G	0.02	0.89	0.05	0.61

Table 2
Coefficients for Wake Modeling Equations 19 and 23

	Surface Fit			Curve Fit
ψ_{00}	0.3511237×10^{-1}		b_0	0.0179349
ψ_{01}	0.1255308×10^{2}		b_1	2.576580
ψ_{02}	-0.4796241×10^{2}		b_2	-2.3062584
ψ_{03}	0.6732523×10^{2}		b_3	0.8951468
ψ_{04}	-0.3572466×10^{2}		b_4	-0.1758604
ψ_{20}	-0.1890581		b_5	0.0169970
ψ_{21}	-0.9345507×10		b_6	-0.0006404
ψ_{22}	-0.1821427×10^{3}			
ψ_{23}	0.5617911×10^{3}			
ψ_{24}	-0.3995373×10^{3}			
ψ_{40}	0.2649465			
ψ_{41}	-0.9434068×10^{2}			
ψ_{42}	0.1034830×10^{4}			
ψ_{43}	-0.2348153×10^{4}			
ψ_{44}	0.1510437×10^{4}			

Source: (12)

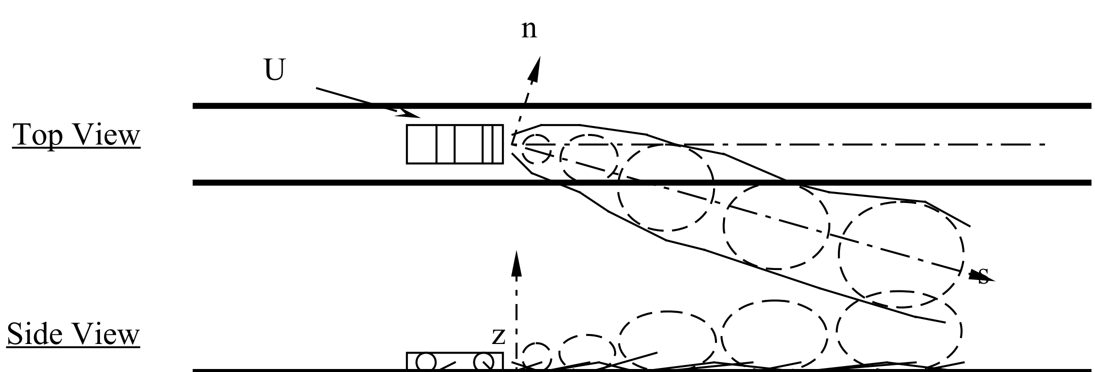
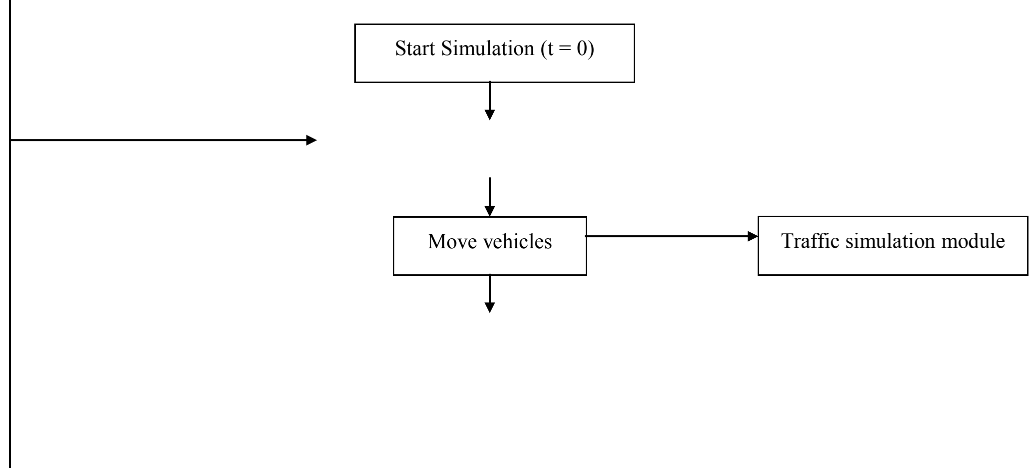


Figure 1
Simplified View of a Wake Behind a Vehicle



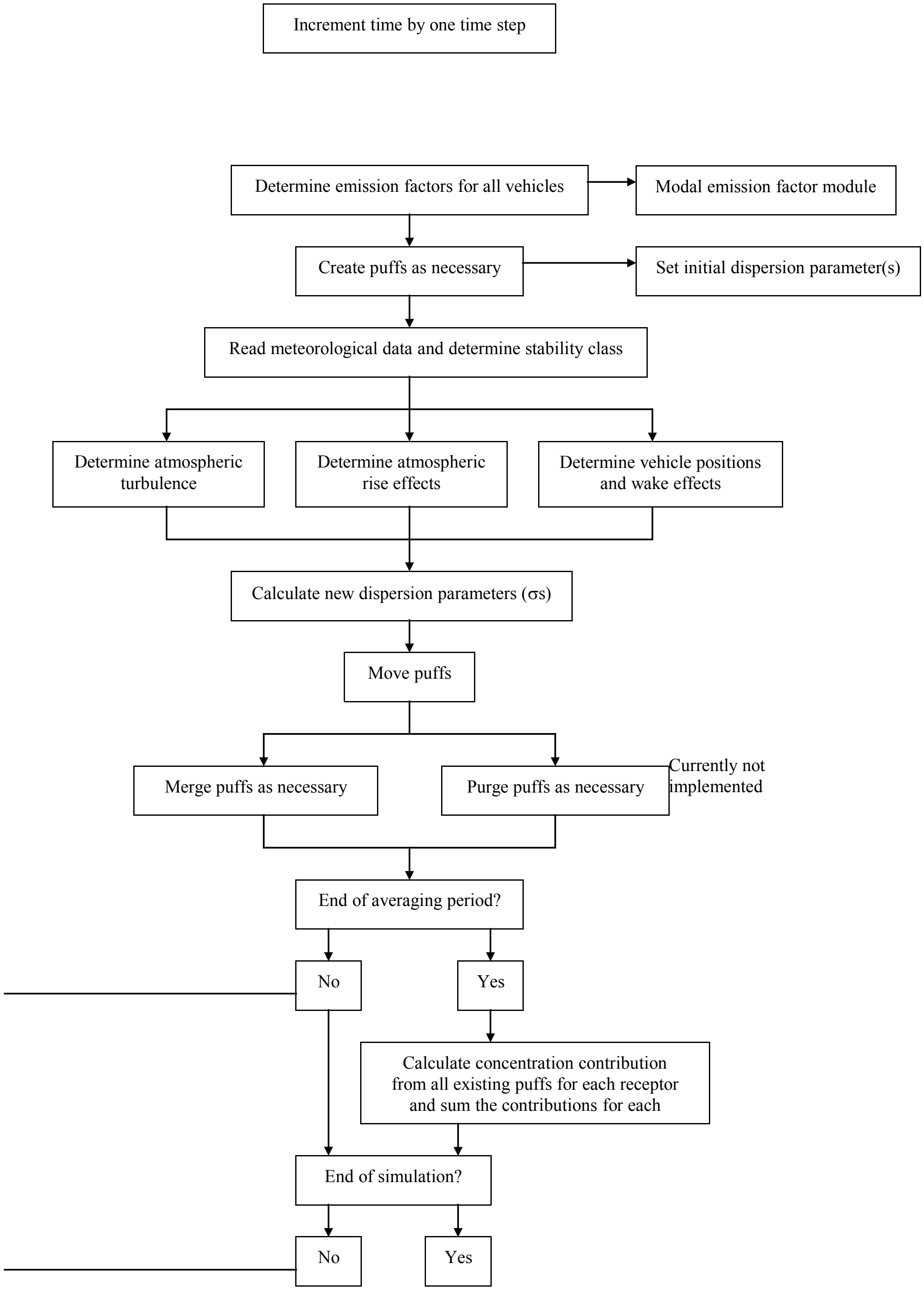


Figure 2
Model Simulation Scheme