CFD modeling vehicle exhaust dispersion in complex urban areas

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Abstract: This work proposes a CFD model for predicting vehicle combustion exhaust propagation in the micro-scale approach, in which the buildings and street canyons in urban areas are accurately represented in computational domain. The pollution dispersion is calculated with the advection-diffusion-reaction equation. The Reynolds averaged Navier-Stokes equations are numerically solved for wind flows. The movement and the heat release rate of the vehicles on the roads are considered as sources for environmental turbulent energy. Two formulations are proposed to represent the light and heavy traffic, respectively. The pollution sources coming from vehicle emissions on the streets may be varied unsteadily, which reflects the movement of vehicles.

Key-Words: Vehicle combustion exhaust; Pollution in urban area; Turbulence generated by moving vehicle; Field model; Finite element method;

1 Introduction
The Gaussian-like methods, widely applied to predict vehicle exhaust distributions in city areas, are based on the two simplifying assumptions: uniform horizontal wind flow, and homogeneous and stationary meteorological turbulence. As a result, the computational data obtained by these methods are quite rough. In many cases they are inadequate to be applied to complex terrain such as urban areas [1]. In order to more accurately predict the details of the pollutant propagation in complex geometric circumstance, some authors employ the Computational Fluid Dynamics (CFD) approach. The CFD approach can represent complex terrains in principle. However, as it is applied to the practical prediction of pollution within the complex urban areas, the estimation of turbulence generated by moving vehicles is still a difficult and open issue. If each vehicle on the roads is accurately meshed like the computations in the published works [8, 16], the prediction of urban area exhaust distribution will lead to a huge computational cost. This is why the CFD approach is currently limited to single vehicle or very simple multi-vehicle cases, or the turbulence generated by the vehicles is neglected [4].

An alternative is to model the turbulence produced by the moving vehicles on the roads so that the details of each vehicle’s flow are not considered but its effect on the pollution propagation is taken into account. Thus, the computational cost is dramatically reduced. This is a practical way to tackle the issue, which is used in this work. The central to this work is the approximation of the turbulent energy rate produced by different moving vehicles, and its implementation in the turbulent kinetic energy equation for calculating the turbulence induced by the vehicles. Thus, a distributed turbulent viscosity and a turbulent diffusivity for pollution are obtained. Therefore the effect of moving vehicles on pollution transport is captured.

2 Problem Formulation
The vehicle exhaust propagation is governed by the convection-diffusion-reaction equation, which reads
\[
\frac{\partial c}{\partial t} + (u \cdot \nabla)c - \text{div}(D \cdot \nabla c) = S
\] (1)
where \(c\), \(u\), \(D\) and \(S\) are, respectively, the concentrations of pollution species, the environmental turbulent averaged velocities, the turbulent diffusive coefficient and the pollution source. The diffusivity of the turbulent fluctuation, according to K-model, can be calculated by [14]
\[
D_t = \frac{\nu_t}{\sigma_t} (m^2 s^{-1})
\] (2)
where \(\nu_t\) and \(\sigma_t\) denote the turbulent viscosity and Schmidt number, respectively.

2.1 Averaged Turbulent Flows
The incompressible Reynolds averaged Navier-Stokes equations (RANS) describe the averaged turbulent flows, in which the Reynolds stress is calculated by Boussinesq constitutive relations.
\[
\frac{\partial u}{\partial t} + (u \cdot \nabla)u = -(\nu + \nu_t) \Delta u + \rho^{-1} \nabla p = 0
\] (3)
\[\text{div}(u) = 0\] (4)

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where \( u \) is the flow velocity vector, \( \rho \) the hydrodynamic pressure, \( \rho \) the fluid density, and \( \nu \) and \( \nu_t \) denote the kinetic viscosity of fluid and the turbulent viscosity, respectively.

### 2.2 Environmental Turbulence
#### 2.2.1 Discrete vehicle model
Let us firstly consider single vehicle case. The velocity of this vehicle on the street is, \( U^{i} = (U_{x}^{i}, U_{y}^{i}, U_{z}^{i}) \), and its initial position is at \( P^{i}_{0} = (P_{x}^{i}_{0}, P_{y}^{i}_{0}, P_{z}^{i}_{0}) \). Thus, at any instant \( t \), the vehicle position may be calculated by

\[
P^{i} = P^{i}_{0} + \int_{0}^{t} U^{i} \, dt
\]  

(5)

The turbulent energy produced by the vehicle consists of two parts: wake turbulence and turbulence generated by heat released exhausting gases. The generation rate of the turbulent energy by the wake can be approximately given by

\[
G_{w}^{i} = c_{d} A \rho \frac{|U^{i}|^{3}}{2}
\]  

(6)

where \( c_{d} \) is the drag coefficient of the moving vehicle, and \( A \) is the cross-section area of the vehicle. The generation rate of turbulent energy by the released heat should equal its releasing heat power, \( G_{h}^{i} \), which can be obtained from vehicle manufacturer.

Since the turbulence generation occurs in the wake area of the moving vehicle, according to the energy conservative principle, at some time instant, these two generation rates are approximated to be distributed in the following form in the computational domain:

\[
G^{i} = \frac{\eta^{i}}{V^{i}} \left[ G_{w}^{i} + G_{h}^{i} \right] \epsilon \frac{4 \pi \eta^{i}}{3} \frac{1}{r^{3}} \left( x-P_{x}^{i} \right)^{2} + \left( y-P_{y}^{i} \right)^{2} + \left( z-P_{z}^{i} \right)^{2}
\]  

(7)

where \( V^{i} \) is the volume of vehicle and \( \eta^{i} \) is a constant which is determined by the requirement: when \( 2r = l^{i} \) (the characteristic length of the vehicle), \( \eta^{i} r^{3} \ll 1 \), means that the source is just distributed in a spherical region with radius \( r \) and the spherical volume equals the vehicle volume.

When there are many vehicles on the roads, say, \( N \) vehicles, the produced turbulent energy by each vehicle can be calculated by the same way as for single vehicle. As a result, the total generation rate of the turbulent energy for the \( N \) vehicles is calculated by

\[
G = \sum_{i=1}^{N} \frac{\eta^{i}}{V^{i}} \left[ G_{w}^{i} + G_{h}^{i} \right] \epsilon \frac{4 \pi \eta^{i}}{3} \frac{1}{r^{3}} \left( x-P_{x}^{i} \right)^{2} + \left( y-P_{y}^{i} \right)^{2} + \left( z-P_{z}^{i} \right)^{2}
\]  

(8)

where \( V^{i} \) is the volume of \( i^{th} \) vehicle.

#### 2.2.2 Continuous vehicle model
In some cases, the amount of vehicles, \( N \), is so large that they can be considered as being continuously distributed. Thus, the generation rate of the turbulence energy caused by the moving vehicles may be calculated by

\[
G_{w} = f N c_{d} A \rho \frac{V^{3}}{2}
\]  

(9)

where \( c_{d} \) is the averaged drag coefficient of the vehicles on the roads; \( A \) is the averaged cross-section area of the vehicles; \( V \) is the characteristic velocity, for example, the averaged driving velocity; and \( f \) is a model coefficient that is less than unity.

The generation rate of the turbulent energy by the released heat is equal to

\[
G_{h} = N \cdot P_{rh}
\]  

(10)

where \( P_{rh} \) denotes the averaged heat release from exhaust of each vehicle. The sum of the generation rates of two types are approximated as a distributed line source in the computational domain. Therefore, we have

\[
G = \frac{\eta}{L A} \left( G_{w}^{i} + G_{h}^{i} \right) e^{-\frac{2 r^{2}}{A^{2}}}
\]  

(11)

where \( L \) is the length of the street, \( \eta \) is a constant which is determined by the following requirement: when \( 2r = l^{i} \) (the characteristic length of the across section of the vehicle), \( \eta e^{-\frac{2 r^{2}}{A^{2}}} \ll 1 \).

#### 2.2.3 Turbulent energy equation
The turbulent energy, \( k \), is governed by the transport equation [11]

\[
\frac{\partial k}{\partial t} + (u \cdot \nabla)k - \nabla[(\nu + \frac{\nu_t}{\sigma_k})\nabla k] = P_{k} + G - \epsilon
\]  

(12)

where \( \epsilon \) is the turbulence dissipation rate and \( P_{k} \) denotes the turbulence production rate by the wind, and \( G \) is the turbulence production rates by the moving vehicles. The turbulence dissipation rate, \( \epsilon \), can be calculated by [11]

\[
\frac{\partial \epsilon}{\partial t} + (u \cdot \nabla)\epsilon - \nabla[(\nu + \frac{\nu_t}{\sigma_\epsilon})\nabla \epsilon] = C_{el} \frac{\epsilon}{k} (P_{k} + G) - C_{e2} \frac{\epsilon^{2}}{k}
\]  

(13)

where \( C_{el} = 1.0, \sigma_\epsilon = 1.3, C_{e2} = 1.44, C_{e2} = 1.92 \).

#### 2.2.4 Turbulent viscosity and diffusivity
Using the \( k \) and \( \epsilon \) distributions, one can easily find the turbulent viscosity

\[
\nu_t = C_{\mu} \frac{k^{2}}{\epsilon}
\]  

(14)
where the coefficient $C_\mu = 0.09$ and the turbulent diffusivity from (2).

### 2.3 Pollutant Source from Vehicle Emission

Similar to the vehicle turbulence computations, two formulations representing the light and heavy traffic on the road have been considered. For the discrete vehicle movements, the point source form is used to define the pollutant sources, which can be written for a single vehicle

$$S^1 = \frac{1}{V_p} k^1 e^{-\xi [(x-P_i)^2 + (y-P_i)^2 + (z-P_i)^2]^{0.5}}$$

(15)

accordingly for $N$ vehicle:

$$S = \frac{1}{NV_p} \sum_{i=1}^{N} k^i e^{-\xi [(x-P_i)^2 + (y-P_i)^2 + (z-P_i)^2]^{0.5}}$$

(16)

where $k$ is the emission rate of each vehicle and $V_p = 4\pi \int r^2 e^{-\delta} dr$. The function, $e^{-\xi [(x-P_i)^2 + (y-P_i)^2 + (z-P_i)^2]^{0.5}}$, is an approximation of $\delta(x-P)$. Consequently, $\xi$, in principle, is a large number, for example, it could be as large as $10^3$ or more. In practical computations we should consider the cell size of meshes. Our experience shows that there exist at least four cells in which $e^{-\xi [(x-P_i)^2 + (y-P_i)^2 + (z-P_i)^2]^{0.5}} > 0.2$. Note that the locations of the point sources are dynamically changed with vehicle movements.

In the second formulation, the pollutant sources for the continuous vehicle distribution case are described as line source:

$$S = (K/V_i)e^{-\delta}$$

(17)

where $K$ is the emission rate of all the vehicles on the street and $V_i = 2\pi L \int r e^{-\delta} dr$ where $L$ is the length of the street. The locations of the line pollutant sources are fixed but the emission rate may be varied with time, which reflects the traffic flux variation with time.

### 3 Numerical Method

The above mathematical problems are numerically solved by finite element method. The employed elements are the hexahedral or/and tetrahedral with tri-linear interpolation functions. Velocity components and pressure are arranged on collocated grid for solution of the Reynolds averaged Navier-Stokes problem. Such collocated arrangement leads to instability of numerical solutions of the Navier-Stokes equations due to violation of the Babuska-Brezzi condition of the saddle point problem. Hence the pressure-stabilizing/Petrov-Galerkin (PSPG) scheme is used to overcome the instability. Another numerical instability comes from solution of convection-diffusion problem, when convective term is dominated in problem. In order to eliminate the second instability, we employ the streamline-upwind/Petrov-Galerkin (SUPG) scheme. There are two parameters in PSPG and SUPG schemes. The exact calculations of the two parameters need to solve a local problem in each element. As an approximation, the simplified calculation, [2], was adopted. The resulting non-linear algebraic system is solved by the Newton iteration method, and the geometrical multi-grid pre-conditionered Krylov iterative method is used for solving the discrete linear algebraic systems in each Newton iteration.

### 4 Computational Results

In computations, the neutral and isothermal atmospheric boundary layer is considered. That means the effect of stratified flow is not considered for the sake of simplicity. The atmospheric density is taken as $1.2kgm^{-3}$ and the free stream turbulent energy is 5%.

The vehicle drag coefficient is assumed as $c_d = 0.15$.

#### 4.1 Exhaust Propagation from One Vehicle

The first case is exhaust propagation from single vehicle on a flat plane without wind flows. The turbulence and emission propagation are yielded only by the vehicle movement. The energy of the turbulent fluctuations is calculated by equation (12) with a source term obtained from equation (8). The computational domain is 5m high, 7m wide and 15m long. In this case, three different vehicle velocity computations, $U = 1.4ms^{-1}$, $U = 2.8ms^{-1}$ and $U = 5.5ms^{-1}$ were considered. Two typical turbulent intensity profiles are displayed in Fig 1: one is along stream direction at central line and the other is across the span direction behind the vehicle. The turbulence produced by lower velocity vehicle is concentrated mostly in the neighbourhood of the vehicle whereas higher velocity vehicle produces a larger and wider region of turbulence.

![Graph](image)
The emission dispersion consists of two components: the convection with the vehicle velocity and diffusion due to the turbulence produced by the vehicle movement. Their dispersion courses are similar. Figure 2 illustrates the pollutant concentration distribution in the middle section. The concentrations profiles behind the vehicle along the central line for the three driving velocities are shown in Figure 3. It can be seen that the maximum concentrations achieve at the position of the vehicle and then rapidly decrease towards downstream.

4.2 Street Canyon Pollution

The second case is vehicle exhaust dispersion in a street canyon. The geometric configuration consists of four cubical building models, 1m wide, 1m high and 20m long, which construct three canyons. A wind flow blows over the buildings and its direction is normal to the building rows. The height of the atmospheric boundary layer is 10 times of the building height and \( \delta = 2ms^{-1} \).

A queue of vehicles is running in the third canyon. The characteristic length of the vehicle is one-tenth of the building height. Two models are used to calculate the exhaust dispersion: discrete point sources and continuous line source. There are 20 vehicles moving with velocity 0.5\( ms^{-1} \) on the street. The major turbulent energy is produced by the moving vehicles in the canyon and it plays an important role for dispersion of the exhaust. In order compare the two models of discretely and continuously distributed sources, the typical turbulent energy profiles by the two models are shown in Figure 3. It is found that the continuous line model gives larger turbulent energy over the discrete point model. This will leads to a stronger dispersion of the pollutant, see Figure 4.

In order to investigate differences between two models, three computations were carried out for the different source terms: 20 moving vehicles; 20 static vehicles and a line source with 20 vehicles. Note that the last case (continuous line source) corresponds to the fixed source term, too. The profiles of the concentrations on two sidewalls produced by these three are illustrated in Figure 4. Although the discrete point source model with moving vehicles gives the results similar to those by the continuous line source model, there are some differences between the two models. The continuous line source model produces a stronger turbulence and a stronger dispersion of the pollutant. The case of the static vehicles is significantly different from the other two cases. This is because the turbulent intensity for the
static vehicle case decreases significantly due to lack the turbulence generated by the vehicle movements.

4.3 Pollution within A Group of Buildings

This section presents an application of the proposed methodology to pollution within a group of buildings. Its geometric configuration is provided by CSTB (French Scientific Centre for Building Physics). The characteristic length in this case is building height, which is 50m. The computational domain is meshed by tetrahedral elements and its grid consists of about ten million tetrahedral elements. The building group is situated inside computational domain. The distance between inlet section and front edge of the building group is about 500m and the back edge is located at about 4000m away from outlet of computational domain. Clearly computation cost for this case is beyond capability of an ordinary workstation. So the computational code is parallelised in message-passive program model and was performed on the parallel computer, HPCx at Daresbury Laboratory in the UK.

A wind blows from south to north. In Figure 8 the wind direction is along Y-axis. The computed wind field is normalized and Reynolds number is about $2.5 \times 10^5$ based on characteristic length of building height, 50m. The computed wind field within the building group is comprised by various vortices yielded by complex geometry of computational domain. Figure 5 shows the wind flow in the horizontal section 15m over the ground. The computational results show that an area of strong turbulence fluctuation appears behind the building group. The stronger the turbulence fluctuation, the faster the turbulent diffusion of pollution in the area.

Under this wind field, propagation of the vehicle emission was studied. The exhaust of gases is described by pollution sources which are distributed along main streets within the building group. Their intensity (the emission rate of exhaust gases) varies with time. On 8:00am it reaches peak and on 17:00pm appears the second peak value. The turbulence produced by the vehicles leads to a turbulent diffusion of pollution. The computation simulates propagation of pollutants during 12 hours using 1200 time steps, each time step is taken as 36 seconds. Figure 6 shows normalised concentration distributions of pollutant species at a horizontal section located at 1m high from the ground at 8:00 am. At that instant, the pollutant concentration arrived its maximum. The line in the street centre represents vehicle queue and the pollution sources are located along it. The red area shows pollution “hot-spot” in this building group. Two hour later, on 10:00am, the amount of vehicles on the street become minimal and the pollution source intensity decreases to its minimum level. At this instant the pollution distribution is almost 50 times less than that at 8:00am. This is because wind and turbulence quickly bring the pollution produced during two hours to downwind areas.

![Computed wind field on a horizontal section of 15 meter high from the ground](image1)

![Concentration distribution of pollutant species on section 1meter high from the ground on 8:00 am. The line at street centre represents car queue.](image2)

![Normalised pollutant concentration variations with time at three points; point 1 in central square of building group, point 2 and 3 on right and left sides of building group, respectively.](image3)

Pollutant concentration at some special locations is of great importance. Three such locations were explored. Figure 7 shows the variation of pollutant concentration at the 3 points with time; point 1 is in the central square of the building group, point 2 and point 3 are on the right and left hand sides of the building group, respectively. It is observed that pollution in the central square is clearly higher than at two end sides.
5 Conclusion
A numerical model for prediction of dispersion of vehicle emissions in geometrically complex urban areas was developed. In order to capture the effect of the moving vehicles on the environmental turbulence, two formulations corresponding to light and heavy traffic respectively are proposed as the source terms for the turbulent energy generation. The case studies considered show that such a treatment is both practical and reasonable within the micro-scale approach. The vehicle emission sources are accurately simulated in unsteady situations. The model presented in this work is adequate to predict the pollution distribution and “hot-spot” within a micro-scale. Further comparison with experimental data and large – scale testing are required.

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