A CFD modelling study of reactive pollutant dispersion in an urban street canyon

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Abstract. This study numerically explores the diffusion rules of pollutants in an idealized urban street canyon where photochemical reactions are present in the neighbourhood. The airborne pollutants dispersion and reaction in street canyons are further investigated in this study. There is a relatively tense traffic pollutants release in urban neighborhoods, including nitrogen oxides and hydrocarbons. Photochemical reaction occurs at strong solar radiation, forming photochemical smog and other environment issues. We selected typical O₃ + NO→O₂ + NO₂ reactions. Effects of the pollutant source location on pollutant dispersion and reaction are also investigated. Numerical simulations were conducted on chemically activity reactive air nitrogen oxides in urban street canyons with W (street canyon wide)/H (building height)=1. Provided three different locations from the line source street canyon bottom exhaust nitric oxide diffusion and react with ozone in the free stream. The chemical reaction has a significant impact on the concentration of pollutants in the valley volume.

1. Introduction
The urban environment has gradually deteriorated due to urbanization and industrialization, especially the urban climate and microclimate air environment [1-3]. In the study of the diffusion of pollutants in an urban street canyon, the various gas pollutants in the atmosphere are generally assumed to be passive and could not have chemical reaction activity. However, there are a lot of gaseous contaminants in the atmospheric contaminant that have chemical activity like Nitrogen oxides. The structure of urban street canyons causes gaseous pollution to linger in the streets and accumulate into high density gaseous pollutants [4-5]. The chemical reactions that occur in the atmosphere are usually reactive occur in short time, which is the time scale of the spread of contamination. Therefore, it could be predicted that there will be pollutant retention in urban street canyon during the chemical reaction, which can be obtained by numerical simulation of the change of pollutant diffusion. There are trace amounts of ozone (O₃) and oxygen (O) in the outer space of cities, which could absorb the sun's harmful ultraviolet radiation [6-9]. But the air pollutants could damage the ozone layer and cause the ozone descend into urban neighbourhood canyons, respectively.

Recently, Computation fluid dynamics (CFD) model simulations [10] has been reported in urban street canyons. We can extend this technology to the prediction of material transport and concentration...
change in the presence of chemical reactions to air pollutants. Bilk [11] used numerical simulation method to simulate the change relationship of air pollutants (NO, NO2 and O3) under photochemical reaction by Large-eddy simulation (LES) model. In the diffusion distribution of pollutants in urban street canyons, the imbalance of chemical reactions in block canyons caused by pollutants in static state was explained. In addition, the Baik has performed a numerical simulation and the navies-stokes equation (RANS) model to analyse the flow of the heated street canyon at the bottom of the street, the study of the effects of the same matter and the effects of the reaction. It is using the RANS model in an existing urban area and Japan also predicts air pollution concentrations. Recently, there have been reports of studies on the air quality of street canyons using photochemical CFD chemical models that take into account O3, nitrogen oxides and volatile organic compounds (VOCs) [12-14].

Although the results showed a bias in previous measurements of NO concentration in China, they also tried to validate their simulations by capturing daily variations in carbon dioxide, nitrogen oxides, and O3 concentrations. In these studies, the feasibility of computational fluid dynamics applications has been demonstrated in predicting the transmission of chemically activity pollutants in urban areas. However, so far, it has not been fully discovered how pollutants react in neighbourhood canyons, which affects pollutant concentrations. In addition to the presence of reaction results in the transmission process of pollutant is non-linear, which keep the relationship between the concentration of the pollutants is particularly important, and the change of the concentration of time special may have great influence on the rate of reaction.

The purpose of this study is to explore existing blocks canyon model of chemical reaction, especially for nitrogen oxides exist before reaction affects the blocks and the mass fraction of gaseous pollutants concentration in the valley.

2. Physical and mathematical models
In this research modelling, the dominant wind direction is prescribed perpendicular to the infinitely long street canyons. Figure 1 depicts the three 2-d block canyon models we set up. The pollutant source NO diffuses from the bottom of the block canyon, the left side of the bottom and the right side of the bottom, and reacts with the O3 transmitted over the block canyon to generate NO2 and O2. We're setting up a neighbourhood canyon that's a block canyon model of the block of the block of W/H = 1.

![Figure 1](image.png)

**Figure 1.** Three different pollution sources placed in the neighborhood canyon model.

In the atmosphere of a normal neighbourhood canyon, there are many things that are reactive, and they may have to be connected through countless reactions. There are pollutants from traffic exhaust in the neighbourhood canyons, especially nitrogen and oxygen compounds. There are many reactions and a series of chemical reactions. These substances could be changed by solar radiation or photodecomposition reactions. Therefore, the aim of this study is to reveal the migration and diffusion rule of pollutant diffusion under the condition of turbulence model [15-16]. What is described in
equation (1) is the only chemical reaction that we set up in a block canyon for numerical calculations:

\[ \text{NO}_2 + hv \rightarrow \text{NO} + \text{O}_3 + \text{NO} \rightarrow \text{O}_2 + \text{NO}_2, \text{O} + \text{O}_2 + \text{M} \rightarrow \text{O}_3 + \text{M} \]  

(1)

where M represents a molecule that absorbs excess energy [17] and k are the kinetics constants as a function of the UV light irradiance [18].

Pollution NO concentrations of our given numerical is \(1.875 \times 10^{-5} \text{ kg/m}^3\). S, the concentrations of canyon is based on the typical city blocks of the material quality concentration the assumption of a given value. Described in total package reaction mechanism of chemical reaction process, solving the transport equation of chemical composition, to solve the local time, on average, the mass fraction of the components that \(m_j\), component j source term (to produce or consume) is a mechanism of all k in the net reaction rate of a reaction.

\[ R_j = \sum_k R_{jk} \]  

(2)

Here, \(R_{jk}[19]\) a chemical reaction or consumption rate is according to the Arrhenius formula, mixing or vortex broken (the EBU) rate of smaller values, for the blocks in the canyon below the rate of chemical reaction, we take the reaction rate of the second order type to indicate.

\[ R_1 = R_2 = R_3 = -k_B C_1 C_2 \]  

(3)

Which \(K_B\) is the reaction rate in a second-order reaction, and in the block canyon model we set the reaction rate set value of 3.7 \(\times 10^{-1}\) ppm, which is refer to as a reference by Chameides and Stedman in the propagation of the material in the photochemical reaction. Also, we use the Renault average method, which also satisfies energy momentum and material transport equation [20].

2.1. Mathematical description of CFD simulations

The isothermal wind of the entire complex is controlled by incompressible continuity equations and navier-stokes equations. The pseudo-steady-state incompressible Reynolds-Averaged Navier-Stokes (RANS) equations developed to the Renormalization Group (RNG) \(k-\varepsilon\) turbulence model was used in this study, RANS model is an appropriate application in urban street canyon ventilation research. It has certain advantages in economy. The governing equations consist of the continuity,

\[ \frac{\partial \bar{u}_i}{\partial x_i} = 0 \]  

(4)

and the momentum conservation

\[ \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} - \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} \]  

(5)

Here, \(x_i\) the Cartesian coordinate, \(\bar{u}_i\) is the average speed tensor, \(P\) the kinematic pressure. The Reynolds stress \(\bar{u}_i \bar{u}_j\) is modeled by model

\[ \bar{u}_i \bar{u}_j = -\nu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) + \frac{2}{3} \delta_{ij} k \]  

(6)

where \(\nu_t (= C_k k^2/\varepsilon)\) is the turbulent kinematic viscosity, \(\delta_{ij}\) the Kronecker delta, its transport is represented by the mass conservation formulation,
\[
\frac{\partial (u_c)}{\partial x_i} = \frac{\partial}{\partial x_i} (D_i \frac{\partial c}{\partial x_i}) + S_p
\]  

(7)

where \( D_i = \frac{\nu}{Sc_i} \), where \( Sc_i = 0.72 \) is the turbulent Schmidt number) is the eddy diffusivity of the pollutant, \( S_p \) the source term. The RNG \( k-\varepsilon \) includes the transport formulation

\[
\frac{\partial (k_i)}{\partial x_i} = \frac{\partial}{\partial x_i} (\alpha_k \nu_i \frac{\partial k}{\partial x_i}) + P_k - \varepsilon
\]  

(8)

\[
\frac{\partial}{\partial x_i} (\varepsilon_i) = \frac{\partial}{\partial x_i} (\alpha_\varepsilon \frac{\partial \varepsilon}{\partial x_i}) + C_{1\varepsilon} \frac{\varepsilon}{k} (P_k) - \left[ C_{2\varepsilon} + \frac{C_e \eta^3 (1 - \eta) / \eta_0}{1 + \gamma \eta^3} \right] \frac{\varepsilon^2}{k}
\]  

(9)

Here, \( \alpha_k \) and \( \alpha_\varepsilon \) are the inverse effective Prandtl numbers for \( k \) and \( \varepsilon \), respectively. More details about RNG turbulent model can be found in [11-14].

2.2. Numerical modelling validation by the benchmark wind tunnel experiments

With the development of urban blocks, the complex and diverse urban air flow organization, large-scale experimental measurement, scaled wind tunnel experiment and CFD simulation have been used in the study of urban ventilation. However, the accuracy of CFD reliability is not always guaranteed. Therefore, it is necessary to conduct numerical verification for wind tunnel experiments. Brown (2000) in the climate wind tunnel of the US environmental protection agency, the measurement results of high resolution mean and turbulent velocity statistics were obtained around the two-dimensional array of buildings. Seven model buildings with \( H = 0.15 \) m length and width were placed at uniform intervals in wind tunnels. The diffusion of air flow and pollutants in the numerical wind tunnel is simulated by the above numerical method.

The flow, horizontal and vertical is coordinates x, y and z. All flow position parameters are relative to the upstream edge of the first row cube at \( x/H = 0 \). The vertical x-z plane at \( y/H = 0 \). For the validation use case, the criterion can be approximately satisfied with reference to Reynolds number of \( 3 \times 10^4 \).

The turbulent values and average velocity profile in 6 blocks agree well with the wind tunnel measurement results. The field area of the two downstream lines is only slightly different. This is due to the k-\( \eta \) model's failure to predict the cyclic region. The turbulent kinetic energy \( k \) of these lines is shown in figure 2. Although the profile of \( k \) is not quite consistent with the wind tunnel measurement, the size of \( k \) is generally predicted, which is quite consistent with the experimental results.
3. Results and discussion

Figure 2 shows the concentration distribution of NO\(_2\), NO, O\(_3\), and O\(_2\) in the canyon of the block when the source of pollution is placed in the central part of the bottom of the canyon by numerical calculation. By observing, we can clearly see that these pollutants migrate and diffuse. First of all, we can see that the chemical reactions in neighbourhood canyons are relatively rapid. In the neighbourhood canyon of W/H = 1, both reactants and products form a vortex in the neighbourhood that runs along the windward facing back cover. For the reactants NO, O\(_3\), NO with the atmospheric O\(_3\) pollution migration to the block soon after the chemical reaction with it, we could see from the figure NO mass fraction gradually decreased over time. On the other reactant, we could observe that O\(_3\) migrates into the neighbourhood and spreads slowly along the fluid flow direction. When O\(_3\) reacts with pollutant NO at the centre of the bottom of the block, the mass fraction of O\(_3\) varies with leeward. The direction of diffusion of the mass fraction decreases, it is part of O\(_3\) and NO reaction occurred. In the vortices model of transport equation, we set the reaction of NO and O\(_3\) to produce NO\(_2\) and O\(_2\), in which NO\(_2\) and O\(_2\), the two gaseous substances that did not exist in the original canyons, are also generated in the block.

We investigate the distribution and diffusion of two gaseous pollutants O\(_3\) and NO\(_2\) in the canyon with chemical reactions. As shown in figure 4, when we place the sources of pollution respectively on the bottom of the block canyon and the left bottom of the block canyon, We take the centre of the block as the baseline to take the building height H as the abscissa to compare the distribution of gaseous pollutants O\(_3\) and NO\(_2\) at the same time in the central location of the block. First of all, we observe the O\(_3\) concentration distribution. When the NO source is placed at the bottom centre of the block, a considerable part of the O\(_3\) close to the ground reacts with the NO source, while the NO source is placed on the left side of the block canyon On one side, O\(_3\) concentrations are still relatively high near ground and O\(_3\) forms a swirling migration diffusion as the fluid flow continues toward the canyon gorge.
Figure 3. Concentration distribution of NO₂, NO, O₃ and O₂ in the street canyon. (a) The source of pollution was placed in the central part in the street canyon and (b) The source of pollution was placed in the leeward part in the street canyon.

Figure 4. O₃, NO₂ distribution map when pollution sources are placed on the central baseline.

At this moment, near the bottom of NO₂, we found that the NO₂ quickly found its way from the central area at the bottom of the block, that is, the place where the NO source was placed. When the source of pollution was placed on the left side of the bottom, NO₂ was generated and then flowed slowly. Slowly spread to the block, in the block above the gaseous pollutants NO₂ is relatively close to the concentration of the place can be seen. So we know there will be a significant portion of the centre at the bottom of the block. O₃ will react with NO and locate in the left-hand side of the block. Some of the canyons react. After O₃ reacts, only part of the NO₂ will propagate into the street canyon. A large portion of the gaseous pollutant NO₂ accumulates on the left side of the block at the bottom, on the leeward side.
4. Conclusion
Present work has investigated the pollutant propagation, thermal and species transports characteristics, incorporating the effects of flow turbulence, heat and species transportation. The streets are more than W/H = 1.0, which represents the general form of the heart of most cities in the world. The traffic position and its direction to the flow have a great influence on the wind speed nearby.

The pollution mainly comes from the atmospheric hole leading to the ozone to pollute the city and even the block canyon, there are a lot of nitrogen and oxygen compounds exist in the locomotive exhaust in the city streets. So we choose to study the gaseous pollutants O3 and NO2 that have health effects on human beings. As a result, we can see that the occurrence of chemical reactions in neighbourhood canyons has a significant effect on the distribution of gaseous pollutants. In particular, the direction of fluid flow in the neighbourhood greatly affects the migration of pollutants in the neighbourhood Diffusion, the fluid flow along the windward toward the leeward, whether it is an unreacted part O3 or part of the gaseous pollutants generated by chemical reaction NO2 will gradually migrate to the entire canyon, especially on the lee side. By studying the placement of NO sources at different locations and comparing the gaseous pollutants at different baselines, it is still evident that there has been the most significant accumulation of pollutants. We could see that chemical reactions have a considerable pollution hazard to the atmospheric environment in the block.

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