Numerical Simulation of NOₓ and Particular Matter Distribution from Urban Street in Beijing China

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Abstract: In recent years, air quality has been a nation-wide issue in Beijing, China with frequent appearance of haze. Disappointingly, most detectors and sensors are mounted in suburb regions that are over ten kilometers away from the center of Beijing. Additionally, most researches are focusing on a general air flow in large scale instead of a specific community. It is important to be aware of the air quality at living communities in urban areas due to a large population. In this study, computational fluid dynamic (CFD) technologies were used to analyze the distribution of NO_x and particular matter (PM) from urban street in Beijing to evaluate the air quality at a certain building. As most air pollutions are caused by vehicle emissions in urban areas, containing NO_x and particular matters, traffic emissions were considered as the only source of contaminants in this study. Commercial software ANSYS Fluent® was used to simulate a number of dispersion scenarios under different boundary conditions to quantify the pollution level for the selected living environment in Beijing, China. Mass fraction, isosurfaces and streamlines of contaminant were presented to analyze the pollution distribution around the area.

1 Introduction

Urbanization transportation is accelerating in China during recent decades; however, the rapid development raises the economic level as well as pollution level in cities, which has aroused public attention [1]. In urban areas of developed cities with a large population, the air quality is much worse than small towns because of the modern tall buildings that prohibit the straight wind and create turbulence in ground level [2]. Due to the large population, a report mentioned that in China the number of cities under heavily polluted are more than other countries [3]. The major pollutant source in large city is vehicle emission [4]. There are four types pollutant generated by vehicle engines that are CO, Unburned Hydrocarbon (UHC), soot and NOx [5]. NOx is a generic term for the mono-nitrogen oxides NO and NO_2. And particular matters are microscopic solids or liquid matters suspended in the earth's atmosphere. It has been demonstrated that over 75% of NOx and 55% particular matter are from vehicles; besides, the automotive emission has a low discharge height, which is highly influencing the air quality on the ground-level. Hence, the analysis of vehicle emission has practical significance and the effect of other emission source could be neglected when urban area is being focused on [6].

Vardoulakis S has attempted to figure out the pollutant concentration in urban areas during one day and one week [7]. MUST Experiment [8] and the Nantes' 99 Experiment [9] have also presented good patterns about pollution dispersion in a large scale. Both of them have provided a close agreement between simulation results and other validated models. However, most previous works have focused on the air flow and pollutants concentration in large regions instead of the influence on a certain building at ground level. The analysis of pollutants dispersion on large scales could make good predictions on the general pollutants distribution. But it could not precisely predict the effects of pollutants on residential areas. The height of the simulation results and the location of monitored data are also significant to provide valuable information for residences.

In this research, the NO_x and particular matters distribution of crossed streets and concentration of a selected building in a community were both tracked to explore the practical influence of the pollutants on people living areas. As Beijing is a world famous city and has attracted nation attention for its haze issue, the west Third-Ring Road in urban areas was considered as the research domain because it is a typical region through two major streets in Beijing. Due to lack of measurements in urban areas, computational fluid dynamic (CFD) was utilized to present the flow pattern and pollutants distribution based on a three-dimensional model. The commercial software Fluent® was used to conduct this three-dimensional, two phases (gas and solid) steady-state simulation. Buildings were simplified by cuboids neglecting the details of outside surfaces, and the transportation emissions were treated as the only pollutant resources with uniform wind velocities. Transportation

emissions were calculated based on analytical equations with the assumption that the transportation rate was at the upper limit of the nation standard. Simulation models were adjusted by comparing results with validated models through a two-dimensional simulation.

The concentration distribution of NO_x and particular matters in the whole domain during a morning was observed, and the concentration of pollutants around the selected building was analyzed to present the influence of pollutants on residential buildings. Simulation results were compared with nation standard as suggestions to the city development guidelines for the government.

2 Methodology

The main numerical model in this study is K-epsilon turbulence model. In some other similar works, even very recent studies, concerning on the CFD investigation of a fluid flow, they have employed the standard k-ε model as well and reported it could be the best turbulence model in some similar works, especially in terms of computational cost [10]. In this study, the wind flow filed between buildings shows high turbulence intensity. And the averaged Reynold term could be easily solved by standard k-epsilon model. The standard k-epsilon model is used to simulate turbulence, which contains an alternative formulation for the turbulent viscosity and conducts a modified transport equation for the dissipation rate derived from an exact equation for the transport of the mean-square vorticity fluctuation. The modeled transport equations are [11]:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right] + 2\mu_t E_{ij}E_{ij} - \rho\epsilon \quad (1)$$

$$\frac{\partial(\rho\epsilon)}{\partial t} + \frac{\partial(\rho\epsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\frac{\mu_t}{\sigma_\epsilon}\frac{\partial \epsilon}{\partial x_j}\right] + C_{1\epsilon}\frac{\epsilon}{k}2\mu_t E_{ij}E_{ij} - C_{2\epsilon}\rho\frac{\epsilon^2}{k} \quad (2)$$

3 Initial data and assumptions

This paper is focusing on the analysis of the air quality of Western Third Ring-Road area, Beijing. Simulation domain is a square area which has a 200m side length taking the intersection of Huayuan Road as the center. In this area, the NO_x distribution and particular matter have been simulated and compared with nation standard to represent the air quality. The structures in this area are complicated, which contain different types of buildings. Residential building, which is greatly affected by pollutant because of the ventilation by opening windows, will be observed primarily.

The major pollutant NO_x source in this domain is exhausted gas from vehicles in both two roads. From the investigation done by Jiang Meng [12], the data of vehicle flow rate in simulation domain during working days especially traffic rush hours is necessary to analyze the pollution condition. From the 2006 Beijing Statistical Yearbook, it could be seen that the number of vehicle in Beijing is up to 5.43 million in 2014 [13]. In this study, the morning rush hours were considered as the major period to study. The average vehicle flow rate calculated in 2014 is showed in Table 1.

Table 1. Vehicle Flowrate in Simulation Domain in 2014 [13]

Time	Average vehicle flow rate
6:00-7:00	1746
7:00-8:00	2210
8:00-9:00	1081
9:00-10:00	1812
10:00-11:00	1823
11:00-12:00	1812

The vehicle which cannot meet upper emission limit of China IV regulation standard was neglected in this simulation. In addition, driving vehicle which has heavy-duty diesel engine in the crossroad is also forbidden. An assumption will be made that vehicles in Western Third Ring-Road could be considered as those satisfy China IV gasoline engine regulation. According to the regulations standard, the emission should be lower than the level showed in Table 2.

Table 2. China IV Gasoline Engine Regulation Standard [13]

CO(g/kWh)	HC(g/kWh)	NO_x(g/kWh)	PM(g/kWh)
1.5	0.46	2.0	0.02

Considering the transportation condition comprehensively, the engines of vehicle driving in urban area can barely reach full load but low-duty. Due to the exhaust quantities of family cars are not larger than 2.5 liters per vehicle generally, it is reasonable to assume that the power of every vehicle is 15 kW, which could be the basic data for calculating the NO_x amount on the road.

$$Q = nPq/t \text{ [14]}$$

where:
Q: Total Pollutant Generation Rate
n: Number of Vehicle
P: Power of Vehicle Engine
q: Pollutant Generation Rate
t: Time

From the equation above, the pollutants generation rate in the crossed roads are showed in Table 3 and Table 4.

Table 3. NO_x Generation Rate in Simulation Domain

Time	NO_x in Working days(kg/h)
6:00-7:00	52.38
7:00-8:00	66.30
8:00-9:00	32.43
9:00-10:00	54.36
10:00-11:00	54.69
11:00-12:00	54.36

Table 4. PM Generation Rate in Simulation Domain

Time	PM in Working days(kg/h)
6:00-7:00	0.52
7:00-8:00	0.66
8:00-9:00	0.32
9:00-10:00	0.54
10:00-11:00	0.55
11:00-12:00	0.54

To analyze pollutants dispersion, wind velocity and wind direction are required. The wind velocity of Beijing is 1.8 m/s in January and is 1.9 m/s in July [15]. The wind direction representation method is using sixteen wind directions based on wind rose, which is the general representation method. In January the wind direction is NNW, and it is SE in July [15].

Since there are plenty of different situations to calculate, a simplification work must be done. From 7:00 am to 12:00 pm during weekdays is the time period which is analyzed in this investigation. January and July, which is the representative of winter season and summer season respectively are selected to obtain the simulation data. The contaminants generation rates and boundary conditions in the simulation are showed in Table 5.

Table 5. Simulation Parametric Study Boundary Conditions

Case	Wind Velocity (m/s)	Wind Direction	Time Period	NO_x Generation Rate (kg/h)	PM Generation Rate (kg/h)
1	1.8	NNW	6-7	52.38	0.52
2	1.8	NNW	7-8	66.30	0.66
3	1.8	NNW	8-9	32.43	0.32
4	1.8	NNW	9-10	54.36	0.54
5	1.8	NNW	10-11	54.69	0.55
6	1.8	NNW	11-12	54.36	0.54
7	1.9	SE	6-7	52.38	0.52
8	1.9	SE	7-8	66.30	0.66
9	1.9	SE	8-9	32.43	0.32
10	1.9	SE	9-10	54.36	0.54
11	1.9	SE	10-11	54.69	0.55
12	1.9	SE	11-12	54.36	0.54

This paper will focus on the pollution level of different surfaces of the residential building at both windward and leeward in different months under morning rush hours. And then the pollutant concentration will be compared with the Ambient Air Quality Standards of China that the NO_x concentration in urban area must be under 250 $\mu g/m^3$, the concentration of PM2.5 must be under 35 $\mu g/m^3$, and the concentration of PM10 must be under 50 $\mu g/m^3$ by one hour average measurement method [15]. In addition, pollutants moving velocity and concentration in the whole domain have also been observed.
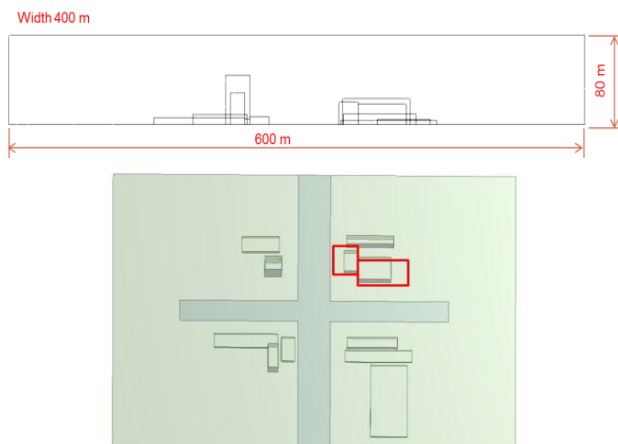

Figure 1. Simulation geometry of the intersection of Huayuan Road in Beijing

The research domain in this study is a square domain which has a 200m side length taking the intersection of

Huayuan Road as the center in Beijing. The detailed simulation geometry is shown in the Fig. 1. This is a three-dimensional domain with several buildings around the sides of two main streets. The mesh for this geometry is around one million elements using both structural mesh for most parts and unstructured mesh for the domain around buildings. The red marked building in Fig. 1 is the research target because it is a living building in a big community with a large number of people affected by the pollutants every day. The simulation solver is a double-precision pressure-based solver with that the relaxation factors for pressure, velocity, and turbulence are 0.3, 0.9, and 0.7.

4 Simulation method and validation

Commercial software FLUENT was used in this study to simulate the contaminants concentration distribution using integrated equations and theories in the software. From the investigation of Efisio Solazzo [16] about the pollutant analysis of Birmingham City in England, a similar model was chosen as the validation of this paper. Base on the geometry in the reference, an optimized model was created, which is showed in Fig. 2. In this model, the inlet boundary and out let boundary were same as those for the model provided by the reference author. The measure line is at the same location as the NO_x monitors in the experiments. Besides, the emission source is the position of vehicle lanes, which are the two directions in both sides. The mesh for this geometry is nineteen thousand elements generated by automated method in ANSYS.
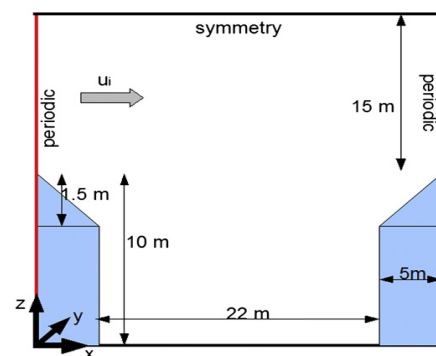

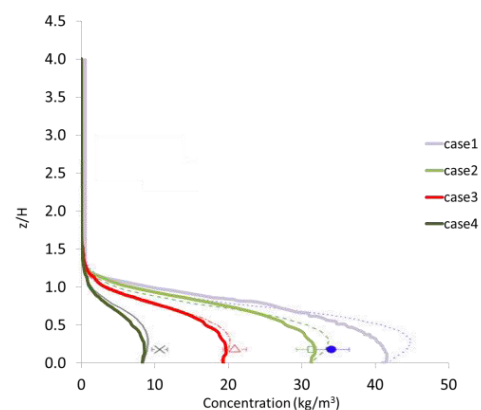**Figure 2.** Optimized validation model [16]

Figure 3. Comparison of simulation results between reference (dash lines) and present study (solid lines)

With the optimized model, using same boundary condition which the reference provided, the simulation of comparison has been conducted. From the result showed in Fig. 3, which has little deviation compared with the data in reference, this simulation model was proved to be credible. The different cases are for contaminant transport under different wind speed in the same wind direction [16].

5 Simulation results

The simulation results were divided into two parts as different conditions in January and July. Both two cases were studied to comprehensively analyze the annual pollution distribution in Beijing. At the same time, the different pollutants emission rates in various time period in one day are also considered to analyze the emission differences during the morning rush hours. In order to compare the results with the standard, the average value during the morning rush hours were calculated to compare to the standard values. As shown in Fig. 4 (a), the wind from north-west with the velocity of 1.8m/s in January was taken as a representative case to evaluate the wind speed changes through the height. As the height increases, the blockage effects of buildings would decrease with the wind velocity increases behind those buildings.

Fig. 4 (b) shows the average NO_x mass fraction distribution at different heights in January. Basically the NO_x distribution is consistent with the wind velocity because the wind motion would be the only force to drive the pollutants movement. As seen in the Fig. 5, the lower height area has higher NO_x mass fraction because it is closer to the emission sources.
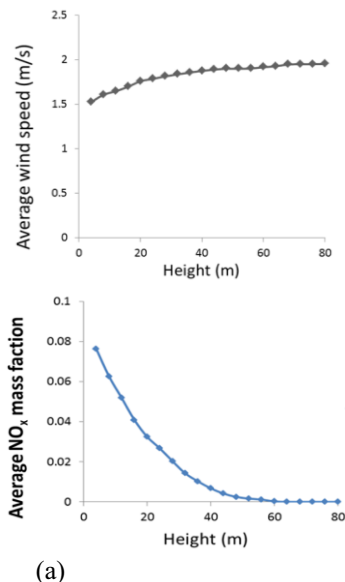

(a)   (b)

Figure 4. Wind speed and NO_x mass fraction distribution in Jan.

As mentioned before, only one of those buildings which are the living building with a large number of people in the big community is the target object in this study. The building is marked by red circle in Fig. 5. It shows the iso-surface when NO_x concentration is 250 ppm. As shown in Fig. 5, the target building is outside the iso-surface, which means the NO_x concentration near the

target building is lower than 250 ppm. The building is not surely affected by the NO pollutants. The table in Fig. 5 also verifies the result that the average NO_x concentrations in different directions of the building are all under the national standard.
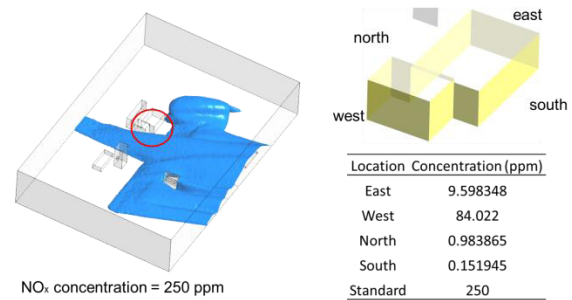

Figure 5. Iso-surface of NO_x concentration during morning rush time in January

From Fig. 6, the particle streamlines are very similar with the NO_x distribution because it is also mainly affected by the wind motion. The average particle concentrations in different directions of the target building are all under the standard that the concentration is 35 ug/m3.
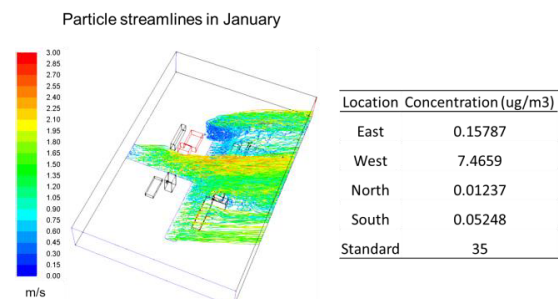

Figure 6. Average PM streamlines during morning rush hours in January

Similarly, the NO_x distribution is also affected by the wind direction in July. And the result is very similar between the case in January and July. As a result, the figures for wind speed and NO_x mass fraction distribution with height changes are not presented here. However, it has an impact on the NO_x concentration near the target building because the wind comes from the direction that the emission pollutants could directly goes into the south surface of the target building.
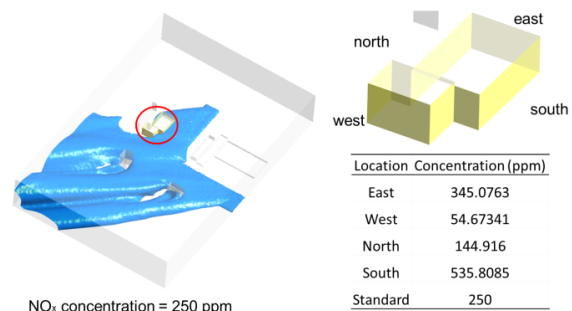

Figure 7. Iso-surface of average NO_x concentration during morning rush time in July

Fig. 7 shows the iso-surface when NO_x concentration is 250 ppm. The target building is inside the iso-surface,

which means the NO_x concentration around the building is over the standard. This condition is different with the condition in January. And from the table in Fig. 7, it is important that the average NO_x concentration of the east and south surface could be much higher than the standard.

From Fig. 8, the particle streamlines are very similar with the NO_x distribution because it is also mainly affected by the wind motion. However, compared with that the NO_x concentration is much higher than the standard, the particle concentration is still safe to people's health in this condition.
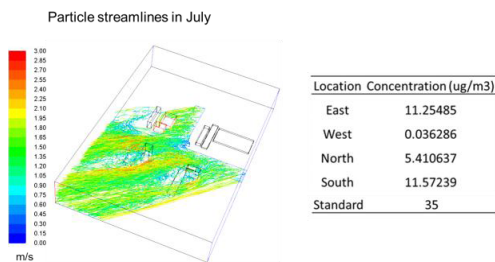

Figure 8. PM streamlines during morning rush hours in July

6 Conclusion

From the simulation results and discussion above, the conclusion can be drawn that the NO_x and particle distribution is strongly affected by the wind direction. For the target building, the surfaces facing the streets which are the emission sources are more likely to be affected by the pollutants. This is guide for people to choose the place where to live and which room to live. Also, the result reminds us of the significance of trees because the blockage to wind has a great impact on the pollutant concentration reaching the building.

Based on the simulation results, another conclusion can be drawn is that the NO_x pollution is highly related to the cars rate and the emission from those cars. However, the particle concentration seems hardly affected by the cars rate because the particle concentration is always under the standard in this study. This could be easily understood relating to the real conditions. Actually the particle pollution is mainly caused by the emission from heavy metal factories and burning grows in specific conditions

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