Modeling of pollutant dispersion in street canyon by means of CFD

Davide Meschini^a, Valentina Busini *^a, Sjoerd W. van Ratingen^b, Renato Rota^a ^a Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano,

^b TNO, Utrecht, Netherlands

Abstract: Nowadays, pollution from traffic remains one of the major sources for contamination in urban areas and it is widely known that substances emitted by vehicles represent a serious hazard to human health; some traffic-related pollutants, such as NO, NO_x and CO are responsible for both acute and chronic effects on human health. This is often the case near busy traffic axis in city centers or street canyons. Purpose of this work is to validate the CFD model predictions against the field measurements of pollutants dispersion in an actual urban environment: Göttinger Strasse, Hanover, Germany. In the location, the population exposure to traffic-related pollution is expected to be high. Steady-state simulations have been performed for 18 different wind directions, with an increment of 20°, in order to cover the whole wind rose. A grid and a Schmidt number sensitivity analysis have been carried out in order to determine both the most suitable resolution of the computational geometry and the most suitable parameter to model the turbulence conditions in the street canyon. All CFD simulations have been performed for neutral atmospheric conditions and have been carried out with the CFD code FLUENT 12.1.

Keywords: CFD, Street Canyon, Atmospheric Turbulence, RANS, Schmidt Number

1. INTRODUCTION

In urban environments, and especially in those areas where population and traffic density are relatively high, human exposure to hazardous substances is expected to be significantly high. This is often the case close to busy traffic axis in city centers or street canyons. The term street canyon refers to a relatively narrow street with buildings lined up along both sides, where prediction of pollutant flow dispersion is particularly challenging because of flow recirculation induced by its configuration.

It is therefore difficult to predict pollutant dispersion with certain accuracy due to the complex interaction between atmospheric flow and flow around buildings. Computational Fluid Dynamics (CFD) techniques are widely utilized to study the wind field and pollutant transport near and around building, because they offer some advantages compared to other methods: they are less expensive than field or tunnel tests and provide results for every point in space. However, this is often accompanied by the difficulty in choosing universal modeling parameters such as the grid resolution and the iterative convergence, in order to obtain reliable results. Moreover, when CFD codes are used to model urban air quality, a proper validation is necessary and the validity of the results is often limited to street geometries and dispersion conditions similar to those for which the validation has been carried out. A difficulty that has been encountered is the fact that field measurements are usually made at a few selected points, which should be representative for the case under examination: for example, it is important to check the presence of concentrations gradients that could mislead the analysis.

The aim of this work is to validate the predictions of a CFD model against the field measurements of pollutants dispersion in an actual urban environment: Göttinger Strasse, Hanover, Germany. In the location, the population exposure to traffic-related pollution is expected to be high. Steady-state simulations were performed for 18 different wind directions, with an increment of 20°, in order to cover the whole wind rose. A grid and a Schmidt number sensitivity analysis were carried out in order to determine both the most suitable resolution of the computational geometry and the most suitable parameter to model the turbulence conditions in the street canyon. All CFD simulations were performed for neutral atmospheric conditions and carried out with the CFD code FLUENT 12.1 [1].

2. MATERIAL AND METHODS

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Typically, there are four boundary conditions required for gas dispersion modeling: inlet, outlet, top and bottom of the computational domain. The analysis was conducted for 18 different wind directions, considering, each time, a change of flow direction of twenty degrees. It has to be considered that the real urban configuration has a 17° -rotation with respect to North. Thus, velocity inlet boundary conditions were applied at two of the four lateral boundaries, while pressure outlet conditions were applied at the remaining two. For wind directions equals to 0° and 180° (i.e. when the wind blows exactly from North or South), symmetry boundary conditions were applied to the lateral boundaries, where no interaction between the borders of the domain and the flow of pollutants is foreseen. At the inlet of the domain the mean wind speed is represented by a logarithmic law instead of a power law in order to generate the initial velocity profile, in accordance with the M-O profile for neutral stratification which states that the mean velocity profile in the lower part of the atmosphere may be adequately described by:

$$u = \frac{u^*}{k} \ln\left(\frac{z}{z_0}\right)$$

where u^* is the friction velocity, k is the von Karman constant (equal to 0.41) and z_0 is the aerodynamic roughness (equivalent to the height at which the wind speed is zero) and assumes different values if related to the buildings or to the terrain: in the first case the value is set at z_0 = 0.01m; in the latter case this changes to z_0 = 0.05m. The logarithmic law is strictly valid only in neutral conditions (i.e. when the temperature profile in the surface layer is closed to adiabatic).

The parameters k_s (sand-grain roughness height) was determined from a relationship developed by Blocken and co-workers [2], as:

$$k_s = \frac{9.793 \cdot z_0}{C_s}$$

where C_s is a roughness constant, set equal to 9.5.

In this work a standard turbulence k- ε model was used [1], which solves the Reynolds-averaged Navier-Stokes equations using turbulence terms derived from separate transport equations for the turbulent kinetic energy k and the turbulent dissipation rate ε . This turbulence closure model was chosen because of its relative simplicity and reliability. The CFD code produces a steady-state solution for the mean flow components and the turbulence variables k and ε . Second-order discretization schemes were used to increase the accuracy of the numerical solution.

3. RESULTS AND DISCUSSION

3.1. Geometrical Configuration

Göttinger Strasse is SSE-NNW oriented (17° -rotation towards West with respect to North), as shown in Figure 1. It is a busy inner-city street, 25 m wide and has 4 lanes, with a traffic volume of about 30,000 vehicles per day and a high share of trucks (16%). On both sides of the lanes there are complexes of buildings (most of which are joined) with an average height of about 20 m. Hence, the aspect ratio of this canyon is slightly less than one. On the tallest building (32 m) there is a 2 m high mast and on this one, in turn, there is a 10 m high measuring mast. At the top of the mast, wind speed, wind direction and the background concentration of pollutants have been registered. The roadmeasuring point is situated before the NLÖ-building, at a location about 1.5 m high and 1m away from the road edge; also at this point, the wind direction and hourly averaged values of NO, NO₂, CO and Benzene are monitored [3]. The measuring point is located not only in close proximity to the road, but also in a highly structured area of the building of NLÖ; hence, for some wind directions the complex geometry can have a significant impact on the measured concentrations. As for the speed of the cars passing by the monitoring point, no data were available; nevertheless, increase or decrease of the allowed urban speed can be excluded, since the street does not present any slope. This means that neither the cars heading northwards, nor the cars heading southwards will pass the monitor under heavy acceleration or in a deceleration phase.

Figure 1: Orientation of the Göttinger Strasse street canyon and height of surrounding



3.2. Evaluation of field data

Testing and validation of a CFD code relies heavily on the availability of experimental data, which have to be compared to the output of the CFD simulations. The State Environmental Agency of Lower Saxony operates a permanent monitoring station in this four-lane street canyon. Detailed field data measurements, and specifications of the case, were obtained from the database of the DGXIITMR TRAPOS. From the provided time series for:

- the number of vehicles on each of the four lanes, divided into small vehicles and trucks;
- the wind speed and wind direction at the station at 42m above the street level;
- the concentrations of NO, NO₂, CO and Benzene at the station and on the road.

For the comparison with the model predictions the mean dimensionless concentration c^* [4] was used:

$$c^* = \frac{C \cdot U_{42} \cdot H}{\frac{Q}{L}}$$

where C is the measured concentration referred to the measuring point minus the background load measured on the roof (it has to be underlined that in a city environment with numerous sources and large local concentration differences it is not easy to determine a meaningful background: in case of the Göttinger Strasse the background concentration is measured on the top of the highest building about 32 m above street level), U_{42} is the wind speed at a height of 42 m (where the monitoring mast is located), H is the characteristic height of the buildings (20 m), L = 180 m is the length of the line sources, Q is the source strength in [mg/s] and Q/L is the specific source strength.

To get a value of source strength, Q, the starting point is to estimate the traffic volume throughout the monitoring period: the analysis of time series generates an average daily traffic volume of about 30,000 vehicles, with a truck share of about 16%, as shown in Table 1.

Traffic Lane	Vehicles	Trucks	% trucks
1	352	56	17
2	220	32	14
3	324	58	17
4	350	50	15

Table 1: Hourly traffic load in Göttinger Strasse.

For the calculation of the emission strength of the line sources, emission factors were used; they represent the relationship between the amount of pollution produced and the amount of raw material processed or burned and depend on the following factors:

- the time-varying number of vehicle;
- the truck share;
- the average speed;
- the percentage of vehicles with cold engine.

To obtain an estimate as reliable as possible, continuous traffic measurements, which also separate vehicles into two categories, were used, thus being able to determine the total emission and the emission factors for each category. It has to be noted that, currently, there are several sets of emission factors in use [3]; Table 2 contains the values used for this validation case.

Table 2: Emission factor both for cars (from the German acronym PKW: Personenkraftwagen) and trucks (from the German acronym LKW: Lastkraftwagen).

Benzene		NO _x		СО	
PKW	LKW	PKW	LKW	PKW	LKW
0.075	0.057	1.03	9.6	15.6	4.1

The emission is then calculated for each lane, considering this equation:

$$Q = P \cdot ePKW + L \cdot eLKW$$

Where Q is the emission of one lane in [mg/s], P is the number of vehicles per lane per second, L is the number of trucks per lane per second, ePKW is the specific emission factor of a vehicle in [mg/m·PKW], and eLKW is the specific emission factor of a truck in [mg/m·LKW].

Plotting all the available data together on a single graph some qualitative trend can be identified, as shown in Figure 2.

Figure 2: Normalized hourly mean concentration values as a function of wind direction measured over a period of one year at the street monitoring station Göttinger Strasse in



However, to obtain a meaningful parameter, the measurements that fell within the same interval of wind direction (step of 20°) and grouped together to calculate a mean value, in order to get an average of the emitted pollutant (i.e., NO_x) in that direction. This same procedure was also applied to the wind

speed at 42 m. Figure 3 shows the computed averaged dimensionless concentration c^* for the complete range of wind directions:



Figure 3: Dimensionless concentration from field data.

Furthermore, the wind speed sensitivity analysis reported in Figure 4 shows that the mean concentration trend is representative of all the ranges of velocity considered: hence, even though it is possible to identify 10 different wind speed classes throughout the entire year of measurements, one can assume that the mean wind speed at 42 m floats around 4.6 m/s. Following this reasoning the value of the friction velocity u^* was estimated as:

$$u^* = \frac{U_{42} \cdot k}{\ln\left(\frac{42}{z_0}\right)} = 0.254 \frac{m}{s}$$



3.3. Computational domain

The computational grid represents a replica of the buildings located in Göttinger Strasse in Hanover; the area can be considered an example of a complex urban geometry, where traffic-induced turbulence and whirls around the buildings can affect the dispersion of pollutants emitted from cars. Its dimensions are L x W x H = 740 x 370 x 240 m³ and it is represented in Figure 5.

Figure 5: Computation domain.



In this study, an unstructured hexahedral grid was generated by sweeping faces in the vertical direction, in order to allow full control over the grid quality, size and resolution [5]. The procedure was executed with the aid of the pre-processor Ansys GAMBIT 2.4.6, resulting in a hexahedral grid with about $6 \cdot 10^6$ cells. The range of the cell dimensions is broad: because of the extension of the domain, some parts of the geometry, which are less important for the flow field through the street canyon have a slightly coarser grid, with the width of the cells increasing towards the borders of the domain. Therefore, the whole grid was meshed using the concept of the meshed size function, which allows controlling the size of mesh elements, keeping the elements in the region surrounding the source small in comparison to those farther away. One specific guideline was also taken into account, in order to generate a grid according to the best practice for the CFD simulation of flows in urban environments [6]: the lateral and the top boundaries were set 5H away from the buildings, where H is the height of the target building, to allow a full flow development.

3.4. Analysis of computational data

Figure 6 shows the first complete set of calculations after convergence was reached; it can be noticed that, in the case of wind blowing from west (with respect to the street axis), the pollutant concentration at breath height is higher than in the case of wind blowing from east. This behavior is correctly predicted by the model. However, the model overestimates the concentration of NO for wind directions between 100° and 200° by up to a factor 3. Given the uncertainties related to both the experimental measurements and the input model parameters, this can be considered quite a fair agreement. The same figure also shows the influence of the u* value.



It can be seen that there are no large differences between results obtained using the u^{*} value suggested by Theodoridis and co-workers [7] and the one estimated from the average wind speed.

3.5. Grid sensitivity analysis

Turbulence models performance of flow around buildings is highly dependent on the mesh resolution. In order to understand if a refinement of the computational domain is needed, a grid sensitivity analysis was carried out by replicating the same computational domain with a coarser grid size obtained using the same size functions as in the first case, but different growth rate and maximum size of the cells.





Figure 7 shows that no significant differences can be noticed comparing the first mesh with a coarser one.

3.6. Schmidt number sensitivity analysis

Another important input parameter is the Schmidt number, which is defined as the ratio of the turbulent momentum diffusivity v_t and the turbulent mass diffusivity D_t :

$$Sc_t = \frac{V_t}{D_t}$$

No universal value of Sc_t can be established and empirical values have been used in different studies: Flesch [8] reported estimated values of Sc_t ranging from 0.18 to 1.34, based on field observations under different atmospheric stability classes and wind conditions [9]. Regarding dispersion around buildings, the results with $Sc_t = 0.3$ show values of concentration, which are closer to the experiments. On the other hand, dispersion in street canyon is different from that around a single building, as argued in Hanna et al. [10] and Milliez and Carissimo [11] that suggest a higher value of Sc_t for the flow within a street canyons. In order to see if a modification of the Schmidt number produces changes on the predicted ground level concentrations, two other sets of calculations were performed, without modifying any other parameter but Sc_t , from its default value of 0.7 to 0.3 and then to 0.1, which are in the range of those used in previous studies. What can be noticed overall is that, by reducing the Sc_t , the dispersion of the pollutant increases, leading to smaller values of concentration, which are closer to the experimental findings. This can be explained because a lower Sc_t means that the turbulent mass diffusivity increases, hence leading to an easier mixing between pollutant and air within the street canyon. Figure 8 and Figure 9 show a comparison between field and computational data for a Schmidt number equal to 0.3 and 0.1, respectively:



Figure 8: Comparison between field and computational data for Sc_t=0.3.

Figure 9: Comparison between field and computational data for Sc_t=0.1.



The two figures also confirm the low sensitivity of the model results to the u* value, in agreement with the results reported in Figure 6.

3.7. Extension of the domain

Another attempt was made in order to get further with the analysis and to see if the comparison between field and computational data could be even more improved: the domain of interest was

increased, hence leading to the addition of more buildings, whose goal is to help the wind flow develop before it reaches the critical region, as shown in Figure 10.





Despite the increase of the domain, the number of cells does not increase drastically due to the usage of size functions: the blocks of buildings added around Göttinger Strasse were meshed roughly, since no precise values of concentration are needed at such distant regions from the monitoring point.





Figure 11 shows the influence of extending the computational domain. Overall, an increase in the dimensionless concentration can be observed, which might be due to the effect of the additional obstacles on the wind speed with a Sc_t value of 0.7.

Large changes are noticed if the Sc_t is modified, as previously shown, decreasing its value from the default option of 0.7 to 0.3 and to 0.1, as shown in Figure 12 and Figure 13.

The same figures also confirm the low sensitivity of the model predictions to the u* value.

Figure 12: Comparison between starting and extended computational domain (Sc_t=0.3).



Figure 13: Comparison between starting and extended computational domain ($Sc_t = 0.1$).



4. CONCLUSION

Purpose of this work was to validate a numerical model to predict pollutant dispersion in a urban street canyon (Göttinger Strasse, Hanover, Germany), by comparing its results to field data consisting of one-year measurements, carried out within an European project of pollution modeling in busy innercity streets (TRAPOS: optimization of modeling methods for traffic pollution in streets). The simulations were performed with the commercial software FLUENT 12.1 in association with a preprocessor, GAMBIT 2.4.6, in order to generate the computational domain. Steady-state RANS simulations were conducted for the case under examination. All the CFD simulations were performed for neutral atmospheric conditions. The wind flow was simulated for 18 different directions, with a change of 20° each time: the qualitative agreement was found to be quite fair. Generally, the numerical results overestimate the concentration measured on the ground, but the concentrations trends were found to be similar. A Schmidt number sensitivity analysis was performed, leading to the conclusion that low values of Sc_t, such as 0.3 or 0.1, tend to improve the agreement of the predicted ground level concentrations inside the street canyon.

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