

Original scientific paper*

AIR QUALITY ESTIMATION AND ERROR ANALYSIS

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Abstract. *Air quality in urban areas is being influenced by many factors, mostly anthropogenic. A proper estimation of pollutant distribution is very important for making decisions for air quality improvement. The application of CFD techniques provides the most detailed information about pollutant dispersion. If we consider pollution a problem, the application of CFD techniques is not a solution to the problem, but an estimation tool, which supplies environment protection experts with the necessary data.*

In this paper, the measured traffic intensity is used for defining initial and boundary conditions for the CFD model. To this aim, the COPERT software package was used. Since it is well known that wind characteristics have the largest influence on pollutant dispersion, they were carefully treated. There are two main wind directions in the City of Niš area, so two groups of simulations were done, for each main wind direction separately. The PHOENICS software package was used for pollutant dispersion estimation.

The two simulations were done considering the traffic intensity distribution, one for the morning traffic minimum, and the other for the afternoon traffic maximum, taking the measured wind data into account at the same time. The results of the numerical simulation show good agreement with the measured wind data and CO₂ concentrations. Three turbulence models were compared: the standard k-ε model (SKE), the RNG k-ε turbulence model (RNG KE) and the Chen-Kim modification of the k-ε turbulence model (CHEN-KIM KE). Error analysis was performed on the basis of the comparison of the u and v velocity components and CO₂ concentration with the measured results.

Key words: *Air quality, Measurement, CFD, Turbulence modeling, Error analysis*

1. INTRODUCTION

Since the earliest history, there has been an interest in environment air quality. Unfortunately, the reason for this interest is in the fact that man himself can cause big disturbances with his usually careless behavior. Nowadays one can witness the overall bad environmental conditions in the entire world. Particularly as the consequence of the always increasing fossil fuels usage, especially in traffic, pollutant concentrations are steadily increasing all over the world.

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All of the above clearly points to the need for a precise determination of atmospheric conditions in urban environments, with the hope that a better understanding of the processes occurring in the lower layers of the atmosphere can lead to the solution of pollution problems.

Micrometeorology deals with dispersion processes occurring in the Atmospheric Boundary Layer (ABL) [1,2]. Air movements in urban areas occur in the roughness sub-layer in which the surface friction effects are dominant and cause specific flow patterns in urban street canyons. It is a fact that creating a model giving a realistic and precise state of ABL is not a solution of the problems mentioned, although providing the largest amount of useful data, which can lead to the solution. This points to the importance of this field, which is obvious from the large number of papers reported on this subject.

In the past couple of decades, following the broader implementation of commercial CFD codes, an extensive number of studies have been presented, concerning physics of street canyons and micro scale pollution dispersion. In the beginning, investigations were overly simplified, and usually considered 2D domains [9, 10]. Very soon, the attention turned to idealized 3D problems, namely to the single street canyons [11-13] or isolated buildings [14-16]. As expected, the investigations on arrays or regular groups of buildings followed [7,17-21]. All previous studies can be considered as generic studies [8]. These were followed by applied studies, which consider real building configurations or whole urban areas [5,6,8,22,23]. Many studies used wind tunnel experiments for the validation of numerical results [7,8,14-17,19,21,24]. Some investigations were done on some specific influences on an urban canyon air quality, as traffic [6,7,13,25], geometry (usually intersections) [26], and even plants [25]. In the last decade, the increased power of computers has enabled the implementation of large eddy simulation techniques in pollution dispersion investigations of isolated buildings or street canyons, and even for arrays of buildings [8,19,21,27-29].

In this paper, special attention is given to the traffic induced emission estimations. It is known that traffic is the largest single pollution source, so a proper estimation of the pollutant emission level is of vital importance. The scope of the paper covers the central urban area of the City of Niš, where the traffic induced pollution problems are most likely to occur, as this is the area with the highest traffic frequency. As the reference component, the concentration of CO₂ was chosen for the measurements, as well as for the simulations.

2. MATHEMATICAL MODEL

The estimation of pollution dispersion is relatively difficult for modeling, so special attention was given to properly choosing turbulence models. On the other hand, as the size of the model was relatively big, namely $5 \times 3.2 \times 1 \text{ km}$ (or 16 km^3), and the available computers had limited power, the model could not be too complex. As the physics of the street canyons is relatively well described in the available literature, the aim of the investigation in this paper was to estimate the influence of traffic induced pollution over the urban core of the City of Niš.

The mathematical model used is expressed by

Continuity equation:

$$\frac{\partial(\rho)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (1)$$

Momentum (Navier-Stokes) equations:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i u_j) = \frac{\partial}{\partial x_j}(\tau_{ij}) - \frac{\partial p}{\partial x_i} + f_i \quad (2)$$

Energy equation:

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_j}(j_{ih}) + S_h \quad (3)$$

Passive scalar (CO₂) transport equation:

$$\frac{\partial(\rho c)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i c) = \frac{\partial}{\partial x_j}(j_{ic}) + S_c \quad (4)$$

where ρ is the density, u_i are the three main velocity components, p is the pressure, f_i are the body forces and any additional momentum sources, h is the enthalpy, c is the scalar contaminant and S_h and S_c represent the generation/destruction rate of energy and species, respectively. τ_{ij} is the momentum shear stress tensor, j_{ih} is the diffusion flux of energy transport and j_{ic} is the diffusion flux of species transport.

In the energy equation, the diffusion flux of energy transport term (j_{ih}) includes the energy transfer due to conduction, species diffusion and viscous dissipation. Similarly, in the CO₂ transport equation the diffusion flux (j_{ic}) arises due to the concentration of gradients. Finally, they are calculated as:

$$j_{ih} = \Gamma_T \frac{\partial T}{\partial x_i} - \sum_j j_{ic} (h_j j_{jc}) + \Phi \quad (5)$$

$$j_{ic} = \Gamma_c \frac{\partial c}{\partial x_i} - \Gamma_{ih} \frac{\partial T}{\partial x_i} \quad (6)$$

where factors Γ_T and Γ_c are the diffusion coefficients for the enthalpy (Fourier's law) and species (Fick's law) transport, respectively. The second terms on the right-hand side in Eq. 5 and Eq. 6 represent the energy transport by diffusion of species and the Soret-effect species diffusion transport, respectively. Finally, the term Φ is the viscous dissipation defined as

$$\Phi = 0.5\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \frac{\partial u_l}{\partial x_l} \quad (7)$$

3. NUMERICAL MODEL

As the above equations represent the system of averaged equations, it was needed to implement a turbulent model in order to close the system and to convert the given set of differential equations into algebraic ones, which were solved using the PHOENICS software package, which stands for *Parabolic Hyperbolic Or Elliptic Numerical*

Integration Code Series. It was the first commercial software package, with the first version PHOENICS 81 from 1981.

PHOENICS is based on the finite volume discretization method. A RANS-based mathematical model with implicit pressure formulation is solved in a semi-coupled manner by a variant of the SIMPLE algorithm. The hybrid discretization scheme was chosen together with the k- ϵ turbulent model. As PHOENICS is multi-purpose software, the validity depends on the application. Yet, it can be assumed that the validity is appropriate, having in mind the 40-year long experience.

As the physics of the street canyons is well described in the literature, the aim of the research presented in this paper was to extend the model to the real, complex configuration of the central urban area of the City of Niš. It can be found in the literature [7] that most of the available turbulent models give the similar flow and concentration fields in a street canyon. For pollution dispersion modeling, the turbulence models do not only have to be used for the Reynolds stresses but also for the turbulent scalar fluxes. Three different turbulence models were tested for this study: the standard k- ϵ , the RNG k- ϵ and the Chen-Kim modification of the k- ϵ model. These models are among the most frequently used for air pollution modeling.

The standard k- ϵ turbulence model (SKE). The assumption on which the standard k- ϵ (SKE) model is based implies that once turbulent energy is generated at the low wave number end of the spectrum, it is dissipated immediately at the same point at the high wave number end. In turbulent air flow modeling, and generally speaking, this is not the case because of a vast size disparity between those eddies in which turbulence production takes place and the eddies in which turbulence dissipation occurs [30].

The RNG k- ϵ turbulence model (RNG KE). The Renormalization Group (RNG) techniques are used to develop a theory for the large scales in which the effects of the small scales are represented by modified transport coefficients. The presence of built-in corrections allows for the use of the model in both high- and low-Reynolds-number regions of the flow. This can be an advantage when the wind velocity is high because at high turbulence Reynolds numbers the RNG k- ϵ turbulence model uses the same mathematical formulation as the standard k- ϵ model, except that the model constants are calculated explicitly from the RNG analysis and assume somewhat different values. The accuracy of this model is questionable when the Reynolds number is significantly lower.

The Chen-Kim modification of the k- ϵ turbulence model (CHEN-KIM KE). Turbulence comprises fluctuating motions with a spectrum of time scales, and a single time scale (k/ ϵ) concept embedded in the standard k- ϵ turbulence model is unlikely to be adequate under all circumstances because different turbulence interactions are associated with different parts of the spectrum. The Chen and Kim modification of the standard k- ϵ model introduces an additional time scale (k/G), where G is the volumetric production rate of k. The ϵ production term is divided into two parts, the first of which is the same as for the standard model but with a smaller multiplying coefficient, and the second of which allows the 'turbulence distortion ratio' (G/ ϵ) to exert an influence on the production rate of ϵ .

A comparison of the models was done by means of the relative error e [8]. It compares the measured values K_{EXP} with the numerically predicted values K_{CFD} in adequate points. Values of e for u and v velocity components and CO_2 concentration are given in Table 1.

$$e = \frac{|K_{EXP} - K_{CFD}|}{K_{EXP}} \cdot 100[\%] \quad (8)$$

Table 1 Relative error for u and v velocity components and CO₂ concentration

Relative error [%]	SKE	RNG KE	CHEN-KIM KE
u	8.8	10.3	13.8
v	8.1	7.9	9.8
CO ₂	2.1	1.8	2.1

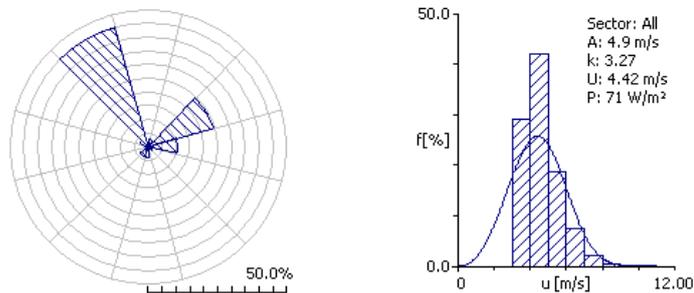
Considering the values of the relative error from Table 1, it is obvious that all turbulent models give relatively similar results. The standard k- ϵ model was chosen as it showed a slightly better prediction of the wind field. The detailed model is presented in Table 2.

Table 2 Standard k- ϵ turbulent model transport equations and constants

Transport equation	Φ	Γ_Φ	S_Φ
Turbulent kinetic energy	k	ν_t/σ_k	$\rho(G - \epsilon)$
Turbulent kinetic energy dissipation	ϵ	ν_t/σ_ϵ	$\rho(\epsilon/k)(C_{\epsilon 1}G - C_{\epsilon 2}\epsilon)$
$G = \nu_t(\partial_k U_i + \partial_i U_k) \partial_k U_i$			$\nu_t = C_\mu k^2 / \epsilon$
$(\sigma_k, \sigma_\epsilon, C_{\epsilon 1}, C_{\epsilon 2}, C_\mu) = (1.0, 1.314, 1.44, 1.92, 0.09)$			

3.1 Boundary conditions for wind

It is known that there are two main wind directions in the City of Niš – North-West ($\sim 330^\circ$, from the Morava river valey) and East ($\sim 90^\circ$, from the Nišava river valey). From the data obtained from the Main Meteorological Station Niš, shown in Fig. 1, it is obvious that there are almost no other wind directions apart from these main two. As measurements were continuously performed, the real wind data were used as boundary conditions. Considering the diagrams shown in Fig. 2, two groups of simulations were done: one for the North-Western wind with the speed of 2.2 m/s and other for the Eastern wind with the speed of 4m/s.

**Fig. 1** Wind rose and Weibull distribution from the Main Meteorological Station Niš

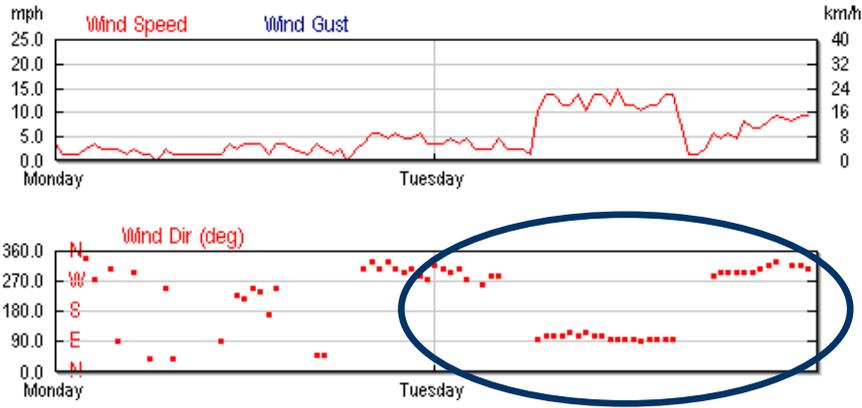


Fig. 2 Wind data for the chosen day

3.2 Boundary conditions for traffic

As for a more proper simulation of the traffic conditions, two traffic scenarios were adopted: the morning minimum, around 6AM, and the afternoon maximum, around 4PM. From the data collected about the frequency of the traffic on the main locations in the city, adequate concentrations were set for each street, considering the counted momentary traffic frequency.

COPERT software was used for the estimation of the emissions on every street. The contribution to the total emission (EC) in $gkm^{-1}s^{-1}$ for each sub-category of vehicles is calculated from the formula:

$$EC = \sum_{i=1}^n \frac{num_i \cdot EF_i}{5 \text{ min}} \quad (9)$$

$$EF_i = a \cdot u^2 + b \cdot u + c \quad (10)$$

EF_i is the emission factor, and u is the average cruising speed in the city, which was found to be 23km/h.

4. RESULTS AND DISCUSSION

4.1 Wind fields

As can be seen in Fig. 3, the maximum wind speed is slightly over 9m/s for the NW wind, and slightly over 10m/s for the E wind, which is in good agreement with the expectations. Average wind speeds are 2.2m/s and 2.7m/s for the NW wind and 3.2m/s and 3.9m/s for the E wind at the height of 1.75m and 12m, respectively. This again shows good agreement with the lower influence of the buildings at larger heights from the ground.

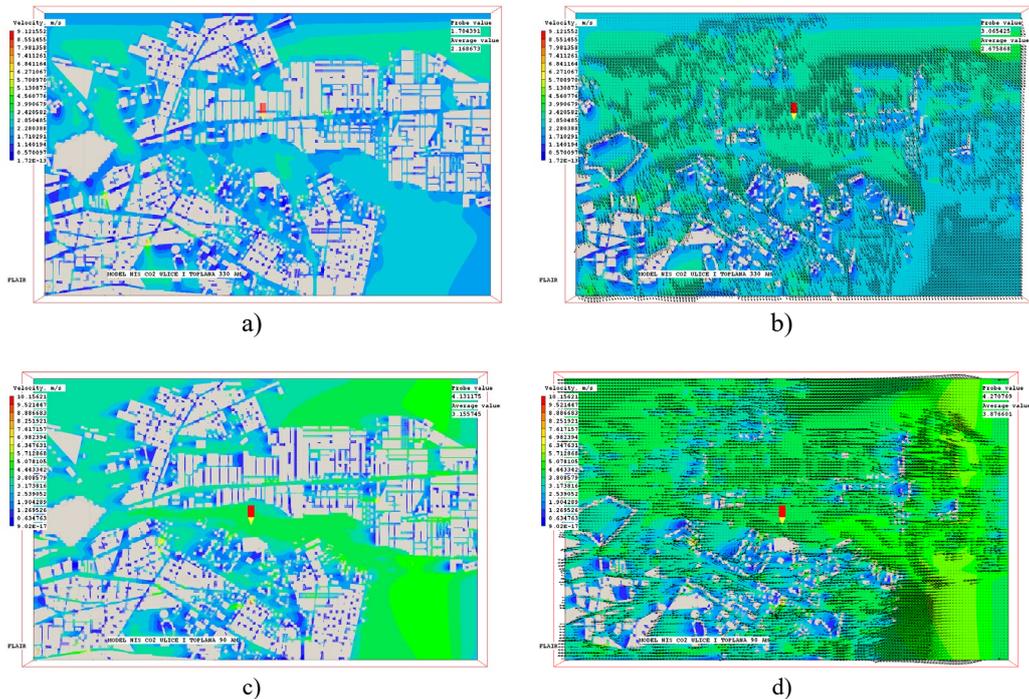


Fig. 3 Wind speed fields for the North-Western wind at the pedestrian head level – 1.75m (a) and above houses – 12m (b), and for the Eastern wind at 1.75m (c) and 12m (d)

It is obvious that the Eastern wind has deeper penetration into the domain, as the river Nišava flows through the middle of the chosen domain in the general East-West direction. Such data were expected, considering the street canyon physics. It can be noticed that the lowest wind speeds are on the bottom of the streets, which is expected, as the objects act as wind shields.

4.2 CO₂ concentration fields

As is well known, the nature of traffic behavior is relatively random. Yet, there are some characteristic points, such as the time when the people are going to work (morning rush hour), and when they are coming back (afternoon rush hour). For the analysis in this paper, the results for the morning minimum (about an hour before the morning rush hour, at 6AM) and at the maximum (the afternoon rush hour, at 4PM) are chosen to be presented. As was previously explained, there are two main wind directions, so the results are shown for each one of them. The fields are presented for the maximum concentrations of 760ppm and 1500ppm CO₂.

As one can notice in Fig. 4, the results are shown for the NW wind direction. Figs. 4a and 4b present the results for the morning minimum of traffic, for the pedestrian head level of 1.75m, and above the houses, at 12m. It can be noticed that the biggest CO₂ concentrations are at the locations of the crossroads with the highest traffic intensity,

mostly in the city center (marked with a red circle in Fig. 4a). Yet, the maximum concentrations are about 700-760ppm CO₂, which are 70-90% higher than the normal atmospheric concentrations.

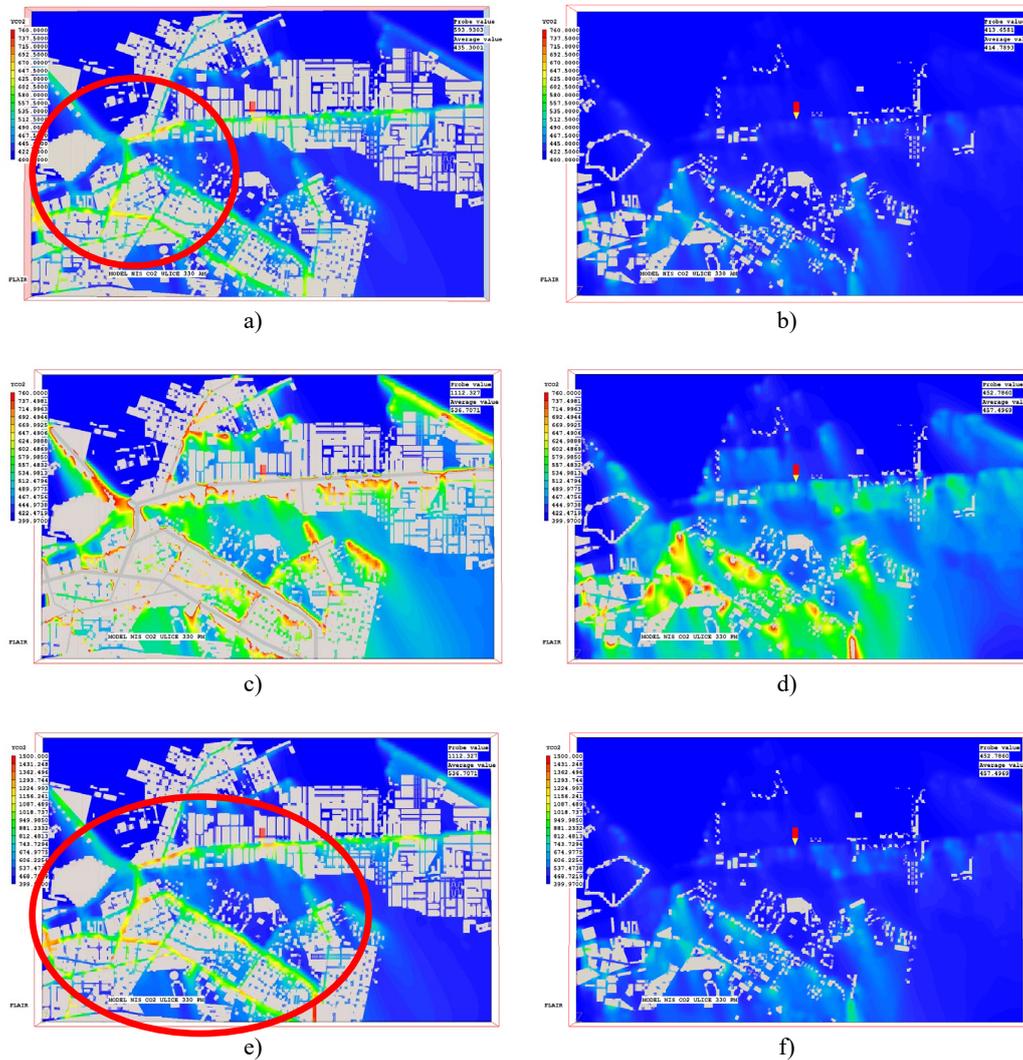


Fig. 4 CO₂ concentration fields for the North-Western wind at 1.75m (a) and 12m (b) at 6AM and at 1.75m (c) and 12m (d) at 4PM for the maximum concentration of 760ppm and at 1.75m (e) and 12m (f) at 4PM for the maximum concentration of 1500ppm CO₂

On the other hand, the situation is getting worse in the traffic peak of the day, as shown in Figs. 4c to 4f. For a better comparison, the same fields are presented for 760ppm and 1500ppm CO₂ maximum concentrations. As can be seen in Fig. 4e, the entire highest

populated zone in the city reaches 3 to 4 times higher CO_2 concentrations at the pedestrian head level, and one can easily notice the actual concentration distribution along the streets.

The results shows that not only crossroads, but the entire length of the streets become places with high air pollutant concentrations. CO_2 concentration distribution is highly affected by the wind characteristics.

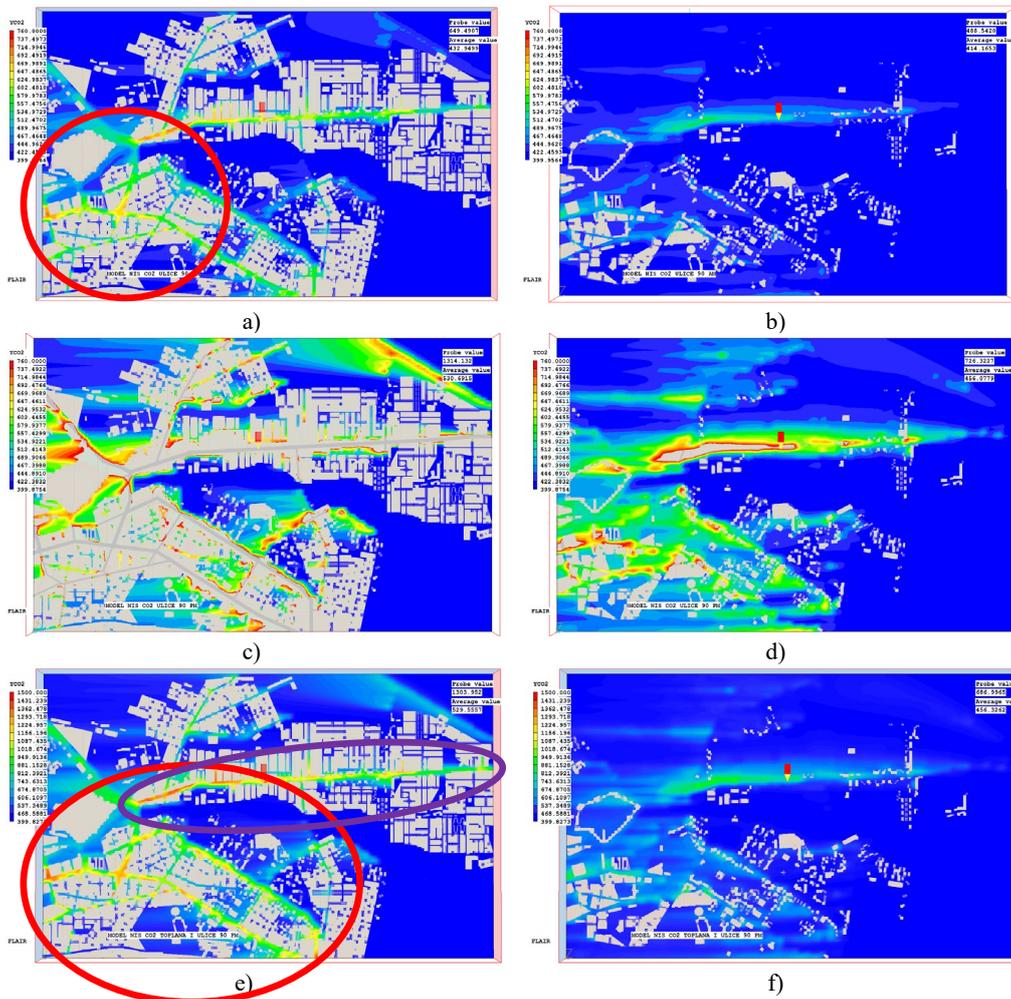


Fig. 5 CO_2 concentration fields for the Eastern wind at 1.75m (a) and 12m (b) at 6AM and at 1.75m (c) and 12m (d) at 4PM for the maximum concentration of 760ppm and at 1.75m (e) and 12m (f) at 4PM for the maximum concentration of 1500ppm CO_2

Similar to Fig. 4, Fig. 5 presents the CO_2 concentration fields for the E wind direction, at the heights of 1.75m and 12m, for the morning minimum and afternoon maximum. As marked with a red circle in Fig. 5a, the morning minimum shows relatively similar CO_2

concentrations inside the street canyons as in Fig. 4a, while Fig. 5b shows a much higher wind direction influence to CO₂ concentration distribution above the street canyons.

For the afternoon traffic maximum, the situation is slightly different. As marked with a red ellipse in Fig. 5e, the zone with high CO₂ concentrations is about the same as in Fig. 4e. The concentration distributions are slightly different, due to the different wind conditions, but they remain at the same level of 3 to 4 times higher than in the normal atmosphere.

The highest difference is for the street marked with a purple ellipse, which is almost parallel to the approaching wind direction. As known from the street canyon physics, in such streets there will be no formation of vortices, and the pollutants will be concentrated in the downwind direction. One can notice that almost the entire street becomes the zone with the highest pollution. The pollution levels are so increased that the downwind lateral streets suffer almost as high concentration levels as the main street, although there is almost no traffic.

On the other hand, one can notice that there is higher penetration of the fresh air along the river as it flows in the wind direction. Such a situation slightly improves the negative pollution accumulation levels for this wind direction.

4.3 CO₂ measurement

As for the need to correctly define boundary and initial conditions for the simulations, the measured results were used for the validation of numerical simulations. The CO₂ concentration is marked with a dark blue line, wind direction with pink, wind speed with yellow and temperature with a light blue line, as shown in Fig. 6. Comparing the measured results with the ones of the simulation for the adequate time, it was found that the CO₂ concentration levels are within the 5% accuracy, which is acceptable, having in mind that the traffic variations for different days are over 10%.

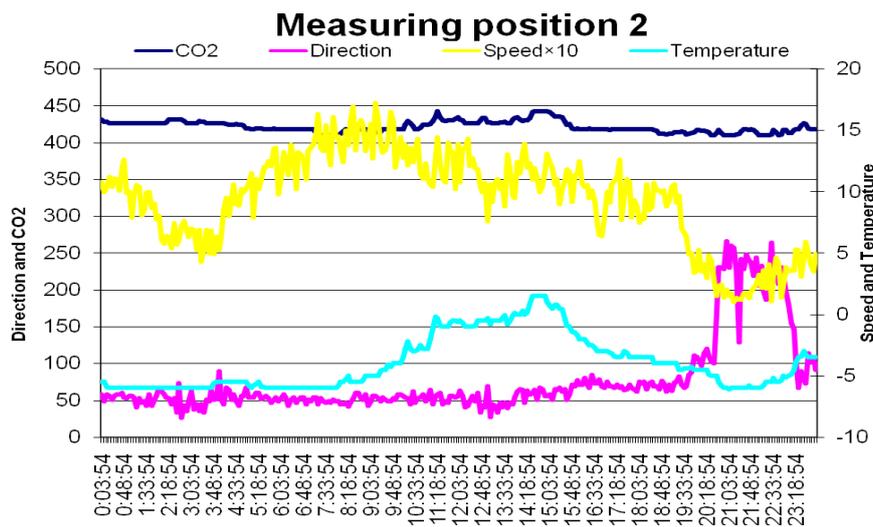


Fig. 6 Data collected on the Measuring site 2 for the chosen day

4.4 Discussion

As the mankind needs for transportation cause a dramatic increase in the number of vehicles that use IC engines, the air pollution in urban areas also increases. The need for a precise definition of the pollution levels in such areas becomes vital for the well-being of the people, as the proper measures can be done in order to prevent a further pollution increase, or to decrease it.

The use of CFD software is one of the possible solutions for improving our diagnostic abilities. The comparison of the current practice of one or a couple of samplings per day, at one or a few locations, with the possibility of continuous measurement and acquiring actual concentration fields, clearly marks the improvements achieved. Moreover, there is a possibility of defining the vertical distribution of the pollutant levels, as shown in Fig. 7. This enables defining the traffic influence not only on pedestrians, but also on the people living on the lower levels in buildings.

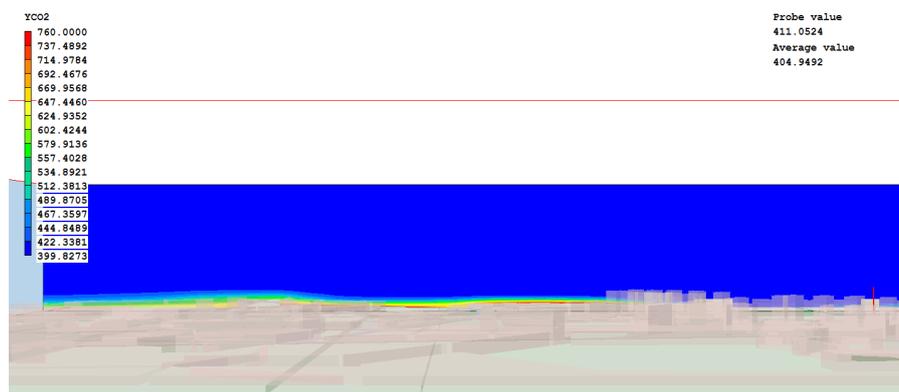


Fig. 7 Vertical distribution of CO₂ concentration

Finally, it can be stated that the CFD techniques are useful tools for defining the pollution conditions in the urban areas. The level of the information available for the environment quality experts is significantly increased, so, it can be expected that they will be used for the overall air quality improvement. In doing so, the life quality of all people living in urban areas will, hopefully, increase.

5. CONCLUSION

A CFD study on air quality in the real configuration of the entire urban core of the City of Niš was performed. Long term measurements were used for defining boundary conditions for wind and traffic. CO₂ was used as the tracer gas, which allowed inexpensive and precise long-term monitoring of pollution levels on several locations in the city. As there are two prevailing wind directions in the City of Niš, the problem could be treated as a steady one in two separate case-studies. For each wind direction, episodes of low (before morning rush hour) and high traffic intensity (afternoon rush hour) were simulated.

Such a specific approach showed the influence of the roads with high traffic frequency on the neighbouring areas with very low traffic frequency. The enlarged concentrations were observed up to 100m from such roads. It is obvious that more studies of real urban configurations are needed, as the pollution problems are increasing. The results obtained from the study can be easily used as a valuable tool in decision-making for further air quality improvement in the real urban area of the City of Niš. It should be noted that this is the first detailed study of this kind in the Republic of Serbia.

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