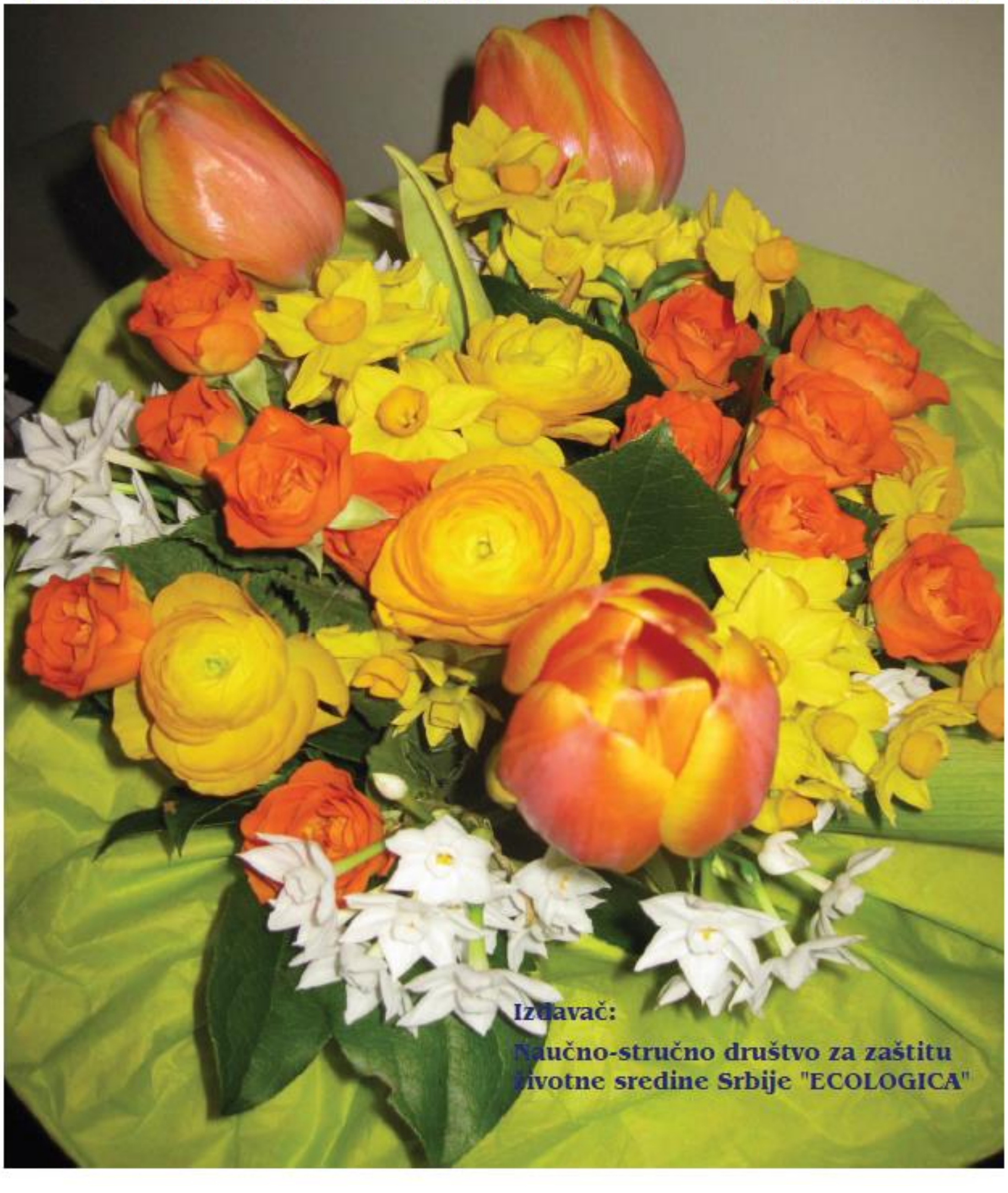
ECOLOGICA

UDC:502.7 ISSN 0354 - 3285

No - 73 • Beograd, 2014. • Godina XXI Samo u pretplati



Izdavač:

Naučno-stručno društvo za zaštitu
životne sredine Srbije "ECOLOGICA"

SADRŽAJ – CONTENT

Numerical simulation of particulate matters and gases pollution dispersion from steel plant in Smederevo

Mirko Kozic[1]
Slavica Ristic[2]
Suzana Polic[3]

Scientific paper
UDC:504.75.054.001.57

INTRODUCTION

Metallurgical industries cause great devastation of both terrestrial and aquatic environments, on a local and regional scale. As indicated, the steelmaking process involves multiple steps, each of which comprises many emissions points. The main sources of pollution in the steel plant environment are: steel plant stacks, open storage yards of mining and fuel, fly ache and slag, and so on. According to [1] the steel industry accounts for 3-4% of total word greenhouse gas emission. Air quality management is a significant segment of the environment protection and it is based on a number of conventions, laws and regulations [2,3]. Determination of trajectories and concentrations of gaseous pollutants and particulate matters is of great importance in protection of human health, ecosystems, industrial or urban areas, historical and cultural heritage [4]. There are many methods dealing with the identification and monitoring of air pollution [5-8].

The last twenty years, one of the methods, which are more and more used to examine air pollution, is numerical simulation. This method takes into account the different parameters depending on the terrain, weather conditions and technical characteristics of the pollution emitter. Software for computation fluid dynamics (CFD) is characterized by high reliability and resolution. Besides, other applications CFD methods are used in ecology to examine the spread of pollutants originating from various sources such as industrial plants, transportation, etc. [8]. The numerical simulation methods are used for solving number problems in metallographic industry. For example, a mathematical model for the four-phase (gas, powder, liquid, and solids) flow in a two-dimensional iron making blast furnace is presented in [9] by extending the existing two-fluid flow models. Numerical simulation applied in industrial practice is presented in [10].The residence time distribution (RTD) of molten steel in the tundish was calculated by mathematical modeling. Inclusion trajectories were calculated using the discrete phase model (DPM) which solves a transport equation for each inclusion particle as it travels through the previously calculated, steady-state, flow field of molten steel and argon gas. In paper [11] FLUENT software was used to simulate the concentration diffusion of dust in an enclosed workshop and ventilation plant, and to analyzed the workshop air velocity, pressure and dust concentration distribution of pollutants.

The investigation of the outdoor air pollution influence on the composition of particulate matter and gases inside the museum of Wawel Castle in Cracow Poland [12], used different methods: combination of micro and trace analysis techniques, EDXRF and EPMA. It is important because the Wawel Castle is located in the centre of Cracow where, in the neighborhood of the city, different heavy industries are located.

One of the pollutant emitter, which has a direct impact on the Smederevo fortress, is the Smederevo steel plant. In spite of implementation of environmental protection measures, which have been conducted over the years, and are being carried out today [13], monitoring shows that there were significantly higher emissions of harmful gases and particulate matters, which is very common in the work of such facilities [2,13-15].

Smederevo Fortress is a monument of exceptional national importance [16]. Due to its complexity it remains today an object of scientific and archaeological interest. The fortress is one of the most monumental architectural buildings from medieval Serbia. Today the Fortress is in a state of

---

Author's address: [1]VTI, Ratka Resanovića 1, Belgrade, [2]Institute Goša, Milana Rakića 35, Belgrade, [3]CIK, Terazije 26, Belgarde, Serbia

Paper received: 20. 01. 2014.
Paper accepted: 01. 02. 2014.

slow, but constant decay, due to many natural and man-made factors (nearby a river port, marina and part of the urban centre of Smederevo, industrial zones, etc). The Smederevo steel plant (recently, U.S. Steel) and several district heating plants, emit CO_2, CO, NO, NO_2, particulate matter, soot, etc. Automatic monitoring of air pollution has been starting in 2007.

This paper presents the results of CO dispersion numerical simulation, emitted from the steel plant stacks. Figure 1 shows the Google terrain map with numerical domain for the simulation of pollution and wind rose in 36 directions; Smederevo1_ Radinac, 2007. year.

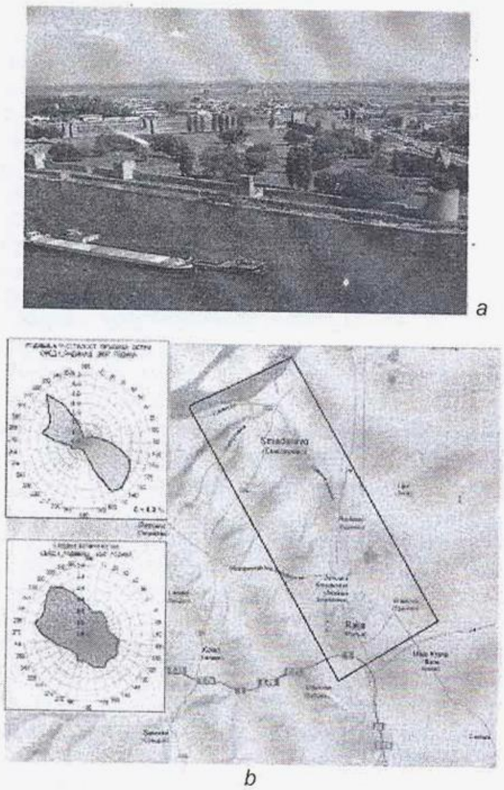


Figure 1 - Smederevo fortress, b- Google map, b- numerical domen and wind rose

1. NUMERICAL SIMULATION OF POLLUTANT DISPERSION

Numerical simulation was performed solving the averaged Navier-Stokes equations of ANSYS FLUENT software package where species transport without chemical reactions was modelled. This model solves conservation equations for chemical species predicting the local mass fraction of each species through the solution of a convection-diffusion equation.

1.1. Pollutants transport equations

The transport and mixing of chemical species are modelled in ANSYS FLUENT [17]. The model includes convection, diffusion and reaction sources for species.

1.1.1. Equations of mass conservation

The local mass fraction for *i*-th species is calculated from general conservation equation given as

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla\bullet(\rho\vec{v}Y_i)=-\nabla\bullet\vec{J}_i+R_i+S_i \qquad (1)$$

Where J_i is the diffusion flux of species *i*, ρ is density of gas mixture, R_i is the net rate of production of species *i* by chemical reaction while S_i is the rate of creation by addition from the dispersed phase.

Mean gas mixture velocity $\vec{v}$ is:

$$\vec{v}=\frac{1}{\rho}\sum_i \rho_i\vec{v}_i \qquad (2)$$

ρ_i is density, $\vec{v}_i$ molecular velocity i- component. Mixture density is:

$$\rho=\sum_i \rho_i \qquad (3)$$

The diffusion flux $\vec{J}_i$ appears when gradient of concentration, temperature and pressure exists. For laminar flow of dilute mixture, $\vec{J}_i$ is the function of concentration gradient:

$$\vec{J}_i=-\rho D_{i,m}\nabla Y_i \qquad (4)$$

Where $D_{i,m}$ is diffusion coefficient, *i* gas component of mixture. For turbulent flow, it must be taking into account the diffusion due to turbulence, that is generally larger than the laminar diffusion and mass diffusion flux due to the concentration gradient becomes

$$\vec{J}_i=-\left(\rho D_{i,m}+\frac{\mu_t}{S_{ct}}\right)\nabla Y_i \qquad (5)$$

S_{ct} is turbulent Shmit number defined as:

$$S_{c_t}=\frac{\mu_t}{\rho D_t} \qquad (6)$$

μ_t i D_t are turbulent viscosity and diffusivity.

The equations of mass conservation are formed by N-1 gas phase, where N is the total number of phases present in the gaseous mixture. Since the sum of mass concentrations for all vapour phase must be equal to 1, that the N-th mass concentration obtained by 1 minus the sum of the mass concentrations obtained by solving the previously formed N-1 equations for the gas phase. In order to minimize the numerical error for the N-th stage is chosen the one that has the largest global mass concentration.

1.1.2. The equation of momentum conservation

Change of momentum equation for the mixture is given in conservative form:

$$\frac{\partial}{\partial t}(\rho\vec{v})+\nabla\bullet(\rho\vec{v}\vec{v})=\rho\vec{f}+\nabla\bullet\prod\nolimits_{ij} \quad (7)$$

where the buoyancy force per unit volume is determined from the expression:

$$\rho\vec{f}=\sum_k \rho_k \vec{f}_k \quad (8)$$

while the stress tensor $\prod_{ij}$ can be written in the frequently used form as

$$\prod\nolimits_{ij}=-p\,\delta_{ij}+\tau_{ij} \quad (9)$$

where τ_{ij} is the viscous stress tensor, given by equation:

$$\tau_{ij}=\mu\left[\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right] (i,j,k=1,2,3) \quad (10)$$

There μ is mixture viscosity.

1.1.3. The equation of energy conservation

In the energy equation for multicomponent mixture the transport of enthalpy due to species diffusion should be taken into account for its significant influence on the enthalpy field.

Equation for the mixture energy conservation can be expressed as a function of enthalpy as

$$\frac{\partial}{\partial t}(\rho h)+\nabla\bullet(\rho\vec{v}h)=-\nabla\bullet\left(\sum_k h_k\vec{J}_k\right)\nabla\bullet\left(\tau_{ij}\bullet\vec{v}\right) -\left(\nabla\bullet\tau_{ij}\right)\bullet\vec{v}-\nabla\bullet\vec{q}+S \quad (11)$$

where h is the specific enthalpy of the mixture, $\vec{q}$ is heat flux, while S includes sources of enthalpy. The first member on the right side of the equation includes the enthalpy transport due to diffusion, and its assessed impact is based on the Lewis number (L). For i-th component of the mixture L is defined by the equation

$$L_{e,i}=\frac{k}{\rho\, c_p D_{i,m}} \quad (12)$$

If the value of the Lewis number significantly different from 1, the neglect of enthalpy transport due to diffusion can lead to significant errors.

1.2. Numerical domain and mesh

The numerical simulation was carried out in the domain that was 11400 m long, 3600 m wide and 1000 m high. The longest side was set at about 25° relative to the south-north direction. The geometry of the ground was generated using digitalized relief [17, 18]. Three stacks of Smederevo steel plant were modelled in pollution dispersion, namely the central agglomeration stack, blast furnaces stack and central stack of steel-making. Height and diameter of the central agglomeration stack were 150 m and 8 m, respectively. The blast furnaces stack was 65 m high with diameter 3.6 m, while height and exit diameter of the central stack of steel-making were 60 m and 3.6m respectively. Smederevo fortress and the stacks can be seen in Fig.2. The fortress was at about 8000 m from the stacks. All the fortress towers were 25 m high, whereas height of all its walls was 10m.

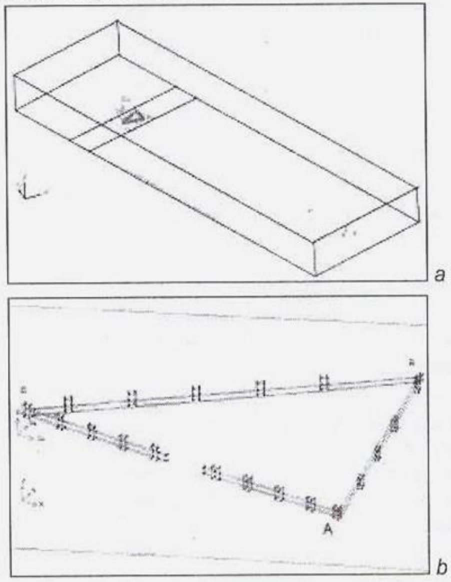


Figure 2 – a) Geometry of the whole numerical domain and b) Smederevo fortress

An unstructured tetrahedral mesh composed of 3 397 961 volume elements was generated. The surface of the ground and fortress were discretized with 388 838 and 61 086 triangular elements. At the exit of central agglomeration stack there was 748 surface elements, while 394 elements were placed at the exits of blast furnaces stack and central stack of steel-making.

The volume mesh in the numerical domain and volume elements in the horizontal plane through the fortress and stacks are shown in Fig.3. There were a large number of small elements near the fortress and stacks because large gradients of the flow field appear in these regions.

1.3. Numerical procedure

Procedure consists of several steps that include modelling transport of multi component mixture and turbulence, selecting the solver formulation, specifying boundary conditions, specifying fluid properties, initializing the solution, monitoring solution convergence, post processing and examining the results.

Boundary conditions at the inlet of the numerical domain were defined with logarithmic profile of the wind velocity. In this way the influence of the ground boundary layer was included. The turbulence kinetic energy and its rate of dissipation at the inlet are not constant, but change as a function of height. Also, the temperature profile was prescribed along the inlet height. The mass fractions of predominant pollutants were specified at the exits of the considered stacks using data from references and measurements of authorized institution [13, 16]. At the exit of the central agglomeration stack and central stack of steel-making the mass fraction of carbon monoxide was $1.1 \cdot 10^{-3}$ and $1.2 \cdot 10^{-4}$, respectively.

The standard k-ε turbulence model was used that includes convection of hot gases and thermal diffusion. This is a semi-empirical model in which transport equations for the turbulence kinetic energy k and its dissipation rate ε are solved. Widespread use of the model is provided by its robustness, economy, and reasonable accuracy for a wide range of fully turbulent flows and heat transfer simulations.

Initially, the first-order accurate numerical scheme was used for reason of the calculation stability. Later on, the calculation was shifted to the second-order accurate numerical scheme. Finally, obtained results were prepared in the form of figures and tables.

2. ANALYSIS OF NUMERICAL SIMULATION RESULTS

The dispersion of gaseous pollutants from the stacks is a function of many factors, most affected by wind speed and temperature gradient. Numerical simulation was performed for a wind speed of 2.9m/s, and the temperature gradient 1.6°C/100m. These conditions correspond to a moderately stable atmosphere and stability class F according to the classification given in [5]. Selected atmospheric conditions are in agreement with data for many years of measurements carried out in the AMSKV Radinac.

2.1. The dispersion of CO

The researches included simulation of CO_2, CO, NO, NO_2, particulate matter and soot diffusion, and in the paper results of CO and NO_2 dispersion are presented. Figure 4a shows the shape of a plume smoke from the stacks to the Smederevo fortress, as well as details of the pollution spreading in the vicinity of the fortress (Fig. 4b). The mass fraction of CO on the walls of the fortress is shown in fig 5. and it is between 10^{-8} and 10^{-7}.

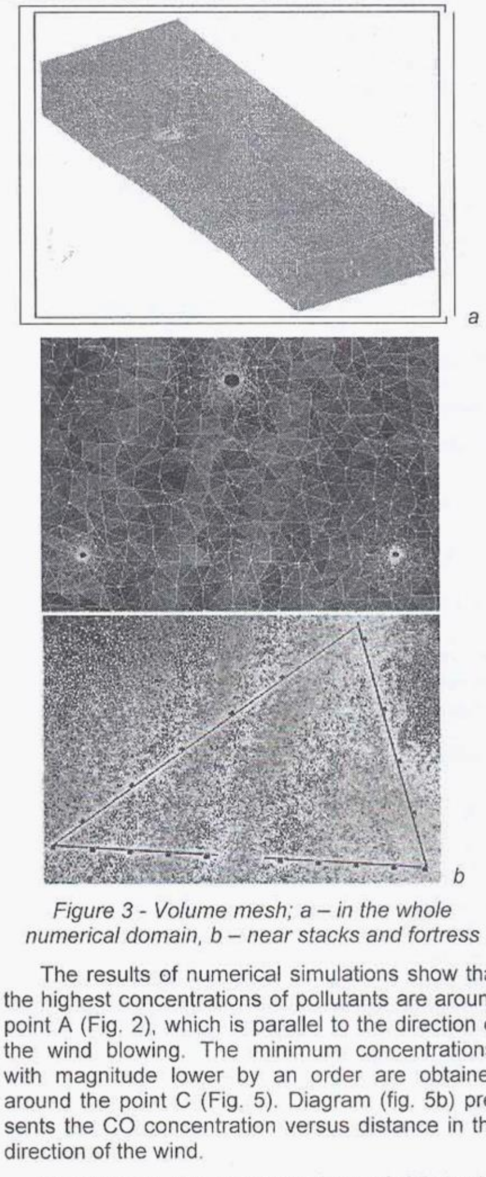


Figure 3 - Volume mesh; a – in the whole numerical domain, b – near stacks and fortress

The results of numerical simulations show that the highest concentrations of pollutants are around point A (Fig. 2), which is parallel to the direction of the wind blowing. The minimum concentrations, with magnitude lower by an order are obtained around the point C (Fig. 5). Diagram (fig. 5b) presents the CO concentration versus distance in the direction of the wind.

In Figure 6, the concentrations of CO in the vertical planes, perpendicular to the direction of the wind blowing are presented. Three planes are set at 900 m, 3700 m and 7000 m from the steel plant stacks, and the last one at 200 m behind the fortress. It can be observed that the fortress is located between the last two planes fig 6a). It is clearly seen that concentration decreases with distance from the stacks.

2.2. The dispersion of NO_2

In Figure 7, the concentrations of NO_2 are presented in the vertical planes, perpendicular to the direction of the wind blowing. The planes have the some locations as the ones for CO presentation; at 900 m, 3700 m and 7000 m from the steel plant stacks, and the last one at 200m behind the fortress. It can be observed that the concentration of NO_2 decreases with distance from the stacks, too.

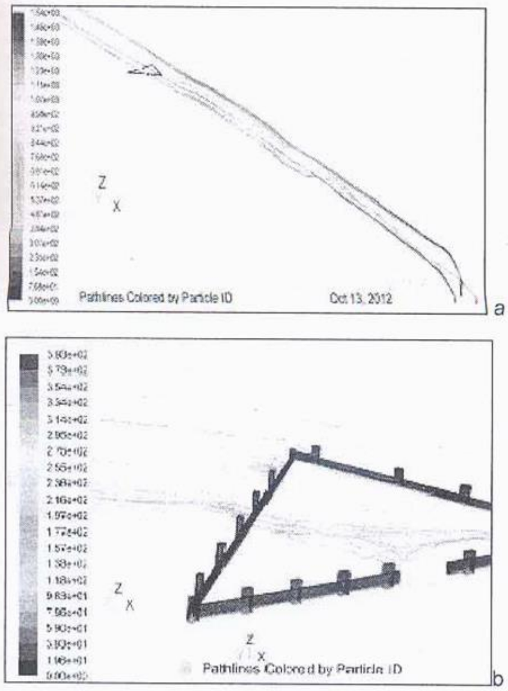


Figure 4 – Traectoris of gaseous pollutants, a-in the whole numerical domain, b-details at the fortress

Obtained results indicate that the mass concentration of NO_2 is in the immediate vicinity of the fortress about 100 times lower ($\approx 2.0 \cdot 10^{-8}$) compared to the mass concentration at the exit of the stack, according to data from the cited literature [13]. On the other hand, the data measured in automated workstation Smederevo centre, located near the fortress [2-4] indicate the following average annual values of NO_2 (2007, 2010 and 2011) respectively: 53μg/m^3 [3, 4] 16μg/m^3 and 19μg/m^3 [2]. Maximum allowable values are to 40μg/m^3 for the period of one year [2].

Measured values for NO_2 concentration are greater than ones emitted from steel stacks, which indicates the existence of more significant sources of this pollutant in the immediate vicinity of the fortress.

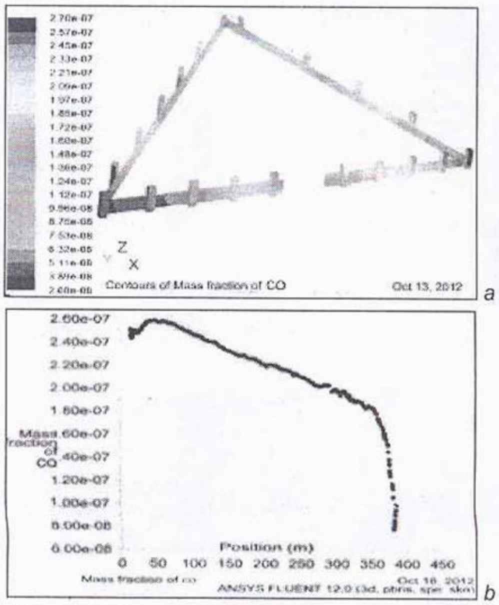


Figure 5 - Concentrations of CO a-at the walls of the fortress, b- CO concentration versus distance in the direction of the wind

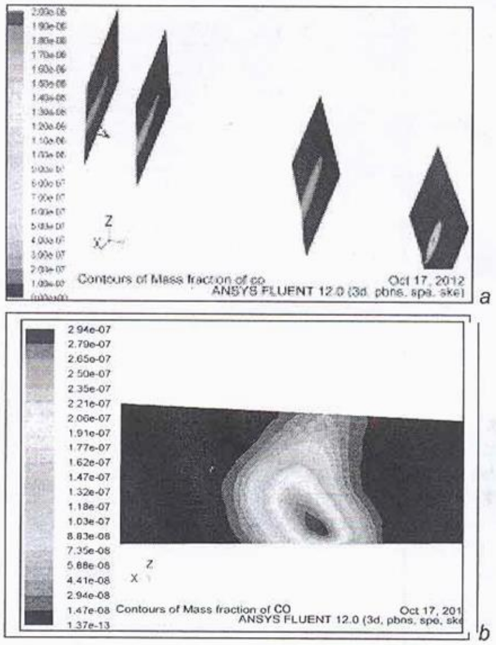


Figure 6 – Concentrations of CO in a-the four vertical planes, b-in vertical plane on the 200m behind the fortress

Figure 8 shows the velocity vectors of the air pollution around the fortress. Details of flow around the walls and towers can be seen in figs 8b and 8c.

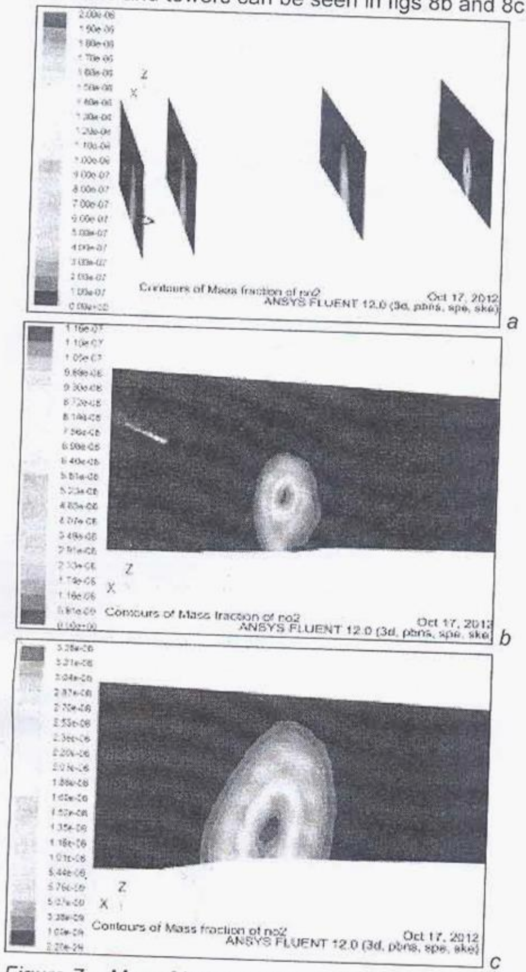


Figure 7 – Mass friction contours of NO_2 in: a- four vertical planes, b-in vertical plane on the 900m from the steel plant stacks c-7000m, d-200m behind the fortress

2.3. The dispersion of particulate matters

Discrete phase model (DPM) is used for numerical simulation of the particulate matter trajectories emitted from the central agglomeration and central stack of the steel plant. The density of particles is chosen to be equal to iron density whereas their diameters are 5 μm, 30 μm and 100 μm.

Figure 9 shows the paths simultaneously from both stacks, trajectory of particulate matters from agglomeration and central blast furnace stack over the whole numerical domain and around the stacks.

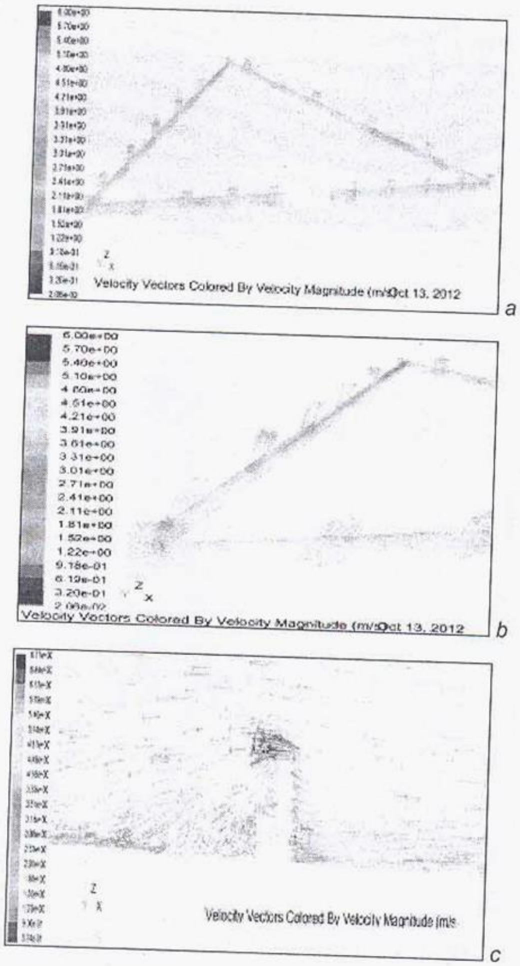


Figure 8 - Velocity vectors around the fortress, b-detail flow around one corner and c- around one of towers

The paths are shown as a function of the particles diameter. Particles with diameter of 100 μm fall to the ground at a distance of several stack height, while smaller ones with diameter 50 μm fly away but without reaching the Smederevo fortress. For given atmospheric conditions the particles with diameter less than 10 μm fly over the fortress.

Results of particulate matter PM10 spread monitoring in the reports of the Ministry of Energy, Development and Environmental Protection data indicate that the highest daily and annual average concentration of particulate matter was measured at station Smederevo-Radinac. For example, in

2011 allowed concentration (>50μg/m^3) was exceeded for 258 days, with an average annual value equal to 85μg/m^3 [2].

Measured values for NO_2 concentration are greater than ones emitted from steel stacks, which indicates the existence of more significant sources of this pollutant in the immediate vicinity of the fortress.

Measured values for NO_2 concentration are greater than ones emitted from steel stacks, which indicates the existence of more significant sources of this pollutant in the immediate vicinity of the fortress.

The numerical simulations of the particulate matters dispersion show that 30 μm particles fall in the vicinity of the automatic air quality monitoring stations in Radinac (fig 9) located at 3 km from the plant (about 2 km in air line). Larger and heavier 100μm particles fall in the vicinity of the steel plant. For considered atmospheric conditions smaller particles reach the city and fortress. Their concentration is lower than at Radinac, but still well above the numerically obtained values.

It means that there are other sources of particulate matter, such as central heating stations, individual coal-fired stoves, and local boiler houses and so on. Heavy rain and strong snowstorm can cause increased pollutant concentration near the ground.

CONCLUSION

Research of pollution dispersion from the stacks of Smederevo power plant and its impact on Smederevo fortress represents the first step in a complex, multidisciplinary approach in analysis influence of industrial zones on cultural heritage objects. Calculation was performed using model of species transport in CFD software.

The sources of pollution considered in the simulation were the central agglomeration stack, blast furnaces stack and central stack of steel-making. The temperature gradient corresponding to inversion was set in the boundary conditions as most unfavourably for level of pollution near the ground. The concentration of carbon monoxide in the vicinity of the fortress obtained by the calculation was about 1 ppm, primarily due to large distance from the stacks that is about 8 km.

The relief of the terrain was included in the model because its influence increases when stack height decreases. Local flow field and level of pollution around the fortress could be changed due to buildings in Smederevo that were not modelled because of limited computer resources.

For a comprehensive understanding of the problem, it is needed to perform identification of all sources of pollution and determine their parameters relevant to the impact on the environment, particularly the objects of cultural heritage. The data collected by the competent institutions in the monitoring process are of great importance. These data are processed by the selected models and used in order to assess the damage and in preventive protection.

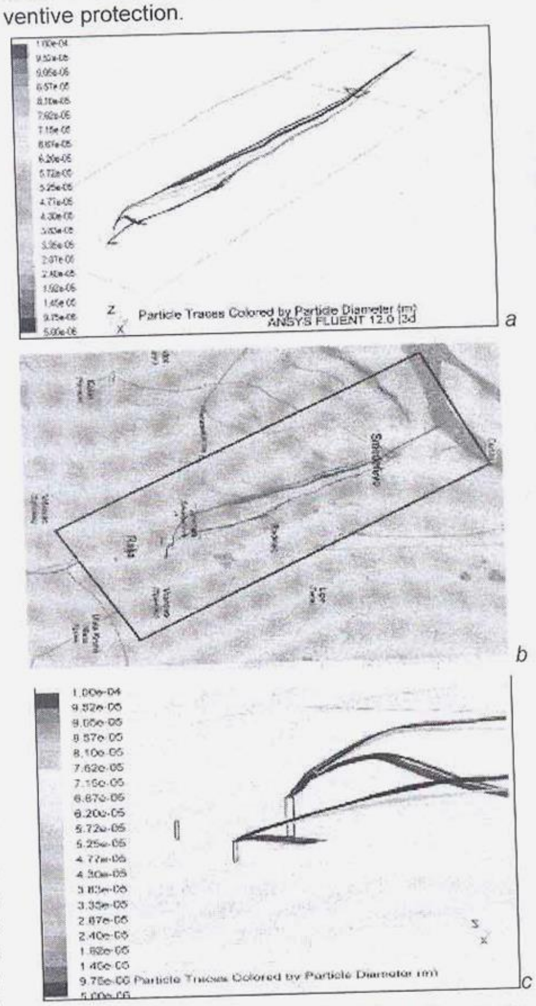


Figure 9. Trajectory of particulate matters from agglomeration and central blast furnace stack, a,b- whole numerical domain, b- part around stacks.

Acknowledgments

This paper is the result of the research within the project TR 34028 and TR 35046, which are financially supported by the Ministry of Education, Science and Technological development and the Ministry of culture and information of Serbia.

REFERENCES

[1] C.C. XU, C. Da-quing, A brief Overview of Low CO2 Emission Technologies for Iron and Steel Making, International Journal of Iron and steel research, 17, 3, 01-07. 2010

[2] Air protection law, ("Sl. gl. RS" br.36/09)

[3] Agency for Environmental Protection, TheAnnual report on the state of air quality in the Republic of Serbia 2011th Belgrade, 2012.

[4] Polic-Radovanovic S., Research unfavourable environmental Impact to the Cultural heritage in Light of International heritological Practice, International Scientific Conference on Environment and biodiversity, ECOLOGICA, Beograd, p.161, 2010.

[5] Pasquill, F., Atmospheric Diffusion, 2nd ed., Halstead Press-Wiley, New York, p.17,1974,

[6] Trini Castelli, S., Anfossi, D. and Finardi, S. Int. J. Environment and Pollution, 40, 1/2/3, 10–25, 2010.

[7] D:L: Doushanov, Control of polution in the iron and steel industry, Pollution control technology, Vol. III,Encyclopedia of Life Support Systems (EOLSS), http://www. Eolss.net/Eolss-sample AllChapiter.aspx

[8] Z. P. Karanıchandan, K. Lohman, C. Seigneu,Using a sub-grid scale modeling approach to simulate the transport and fate of toxic air pollutants, Environ Fluid Mech, 9, 59–71, 2009, DOI 10.1007/s10652-008-9097-0.

[9] X. F. Dong, A. B. Yu, and J. M. Burgess, Modelling of Multiphase Flow in Ironmaking Blast Furnace, Ind. Eng. Chem. Res., 48, 214–226, 2009.

[10] Z. Meijie, G. Huazhi, H. Ao, Z. Hongxi and D. Chengji, Numerical simulation and industrial practice of inclusion removal from molten Steel by Gas bottom blowing in continuous casting tundish, J. Min. Metall. Sect. B-Metall. 47, 2, B 137 – 147, 2011.

[11] T. Lian,W. Wenyong, The Diffusion Simulation of Dust Concentrationin Steel-making Plant, Guangdong Chemical Industry, 12, 2010, http://en.cnki.com.cn/ Article_en/CJFDTOTAL-GDHG201012017.htm

[12] A. Worobieca, Transport and deposition of airborne pollutants in exhibition areas located in historical buildings–study in Wawel Castle Museum in Cracow, Poland, Journal of Cultural Heritage 11, 354–359, 2010

[13] Report on measurements of emissions from the stack steel plant in Smederevo, which was completed Department of Control and Supervision of the Ministry of Environment, Mining and Spatial Planning, in the period since 2006. until the 2010th http//www.balkanphotocontest.comindex.phpmenu=7&img=73743

[14] http://www.ekologija.rs/povecana-zagadjenost-u-okruzenju zelezare

[15] www.tvrdjava.com/ sartid

[16] ANSYS FLUENT 12.0 User's Guide

[17] Raster map 1: 25,000 No. 430-4 (2,4), 2 Digital Terrain Model - grid, the area that includes the Smederevo fortress and U.S. Steel (approx. 16 km2, approximately 8km long and 2km wide) in DXF format, CS Military Geographical Institute, Belgrade, 2012

[18] M.S.Kozic, S.P. Radovanović, S.S.Ristic, Analysis of Air Pollution Dispersion From the Steel Plant in the Region of Smederevo Forteress by Numerical Simulation, (CFD)MME SEE 2013, 23 to 25 May 2013, Belgrade, Serbia., Proceedings, pp.229-235, 2013.

ABSTRACT

NUMERICAL SIMULATION OF PARTICULATE MATTERS AND GASES POLLUTION DISPERSION FROM STEEL PLANT IN SMEDEREVO

This paper presents the results obtained by numerical simulation, of air pollution dispersion from the stacks of steel plant in the direction of Smederevo fortress. Trajectories and concentrations of pollutants (particulate matters, CO and NO_2) were determined by commercial software ANSYS FLUENT. The relief of the terrain was included in the geometry of the numerical domain (11400x3600x1000m). An unstructured mesh composed of more than three million cells was generated. Southeast wind speed was 2.9 m/s blowing in the direction parallel to the longest side of the domain. Atmospheric conditions correspond to conversion, i.e. increase in temperature with height. The sources of pollution included in the simulation are central agglomeration stack, blast furnaces stack and central stack of steel-making. Obtained results represent the first step in a complex, multidisciplinary research of the industrial zones impact on cultural heritage objects.

Key words: *numerical simulation, air pollution, steel plant, Smederevo fortress*

IZVOD

NUMERIČKA SIMULACIJA ŠIRENJA ŠTETNIH GASOVA I ČESTICA EMITOVANIH IZ ŽELEZARE U SMEDEREVU

U radu su prikazani rezultati širenja štetnih materija u vazduhu, emitovani iz dimnjaka železare u pravcu Smederevske tvrđave, dobijeni numeričkom simulacijom. Putanje i koncentracija polutanata (čestica, CO I NO_2) su simulirani komercijalnim softverskim paketom ANSYS FLUENT. Reljev terena je uključen u geometriji numeričkog domena, čije su dimenzije 11400x3600x1000m. Generisana je nestruktuisana mreža sa više od tri miliona ćelija. Numerička simulacija je vršena za jugoistočni vetar (paralelan dužoj stranici domena) brzine 2.9 m/s. Atmosferski uslovi odgovaraju slučaju konverzije, temperatura raste sa visinom. Izvori zagađenja su centralni dimnjak aglomeracije, dimnjak visoke peći i centralni dimnjak čeličane. Dobijeni rezultati su samo prvi korak kompleksnog, multidisciplinarnog istraživanja uticaja industrijskih zona na objekte kulturne baštine.

Ključne reči: *numerička simulacija, zagađenje vazduha, železara, Smederevska tvrđava*