UNIVERSITY OF NIŠ
The scientific journal **FACTA UNIVERSITATIS**
Series: **Mechanics, Automatic Control and Robotics** Vol.2, No 10, 2000 pp. 1243 - 1252
Editor of series: Katica (Stevanovi}) Hedrih, e-mail: katica@masfak.masfak.ni.ac.yu
Address: Univerzitetski trg 2, 18000 Niš, YU, Tel: +381 18 547-095, Fax: +381 18 547-950
http:// ni.ac.yu/Facta

MATHEMATICAL MODELING OF A THREE-DIMENSIONAL ISOTHERMAL SINGLE-PHASE TURBULENT FLOW IN THE CUBIC BOX

UDC 519.87:532.517.4:514.1(045)

Simeon Oka, Srdjan Belošević

Institute of Nuclear Sciences - Vinca, Laboratory for Thermal Engineering and Energy
11001 Belgrade, P.O. Box 522, Yugoslavia

Abstract. *Numerical predictions presented in the paper have been performed as a starting phase in development of 3D mathematical model of a single- and two-phase turbulent flow, with possible application in simulation of processes occurring in power plants and process engineering equipment.*
Turbulent flow of incompressible fluid through the cubic box in isothermal conditions was described by a system of time averaged conservation equations, using the two - equation k-ε model of turbulence and SIMPLE calculation algorithm.
Calculations are compared to the results of measurements taken from the literature. A turbulent water flow enters the cubic box with sides 50 cm, through the square window. The flow impinges the opposite wall, recirculates and moves towards the exit square window in the lower half of the box. Cubic box differs from usually considered cases where dimension in one direction is a dominant one. Flow visualizations were made by using plane light beams and measurements by LDA.
Comparisons are given for a vertical plane going through centers of inlet and outlet windows. Calculated mean velocity vectors satisfactorily agree with measurements. Streamlines in different planes, presented as well, emphasize the complexity of a three-dimensional flow. Predictions for turbulence kinetic energy, given at different axial positions, agree fairly well with measurements.

1. INTRODUCTION

Mathematical models give to both the scientist and engineer a new investigating and designing low-cost tool, having a high reliability and accuracy. It could be used for research, problem solving, assessing changes to plant operating conditions, controlling and designing new plants, taking into account the ever-increasing requirements for efficiency, economy and ecology. Improvements of complex processes with a number of mutual interactions are based primarily upon the fluid dynamics, because the single- and

Received July 2, 2000

multi-phase flows form the very basis of most of physical and chemical processes. Excellent and comprehensive overview of present status and future needs considering mathematical modeling of coal combustion processes can be found in Ref. [1].

Development and step-by-step verification of computer codes give us the opportunity to attain necessary experience and to make the codes developed meet the specific acquirements and needs in the area in which they are to be applied. The present paper gives the results of a three-dimensional single-phase turbulent flow mathematical modeling that should serve primarily as a starting point for development of a complex two-phase model of pulverized coal combustion in real 3D geometry of boiler furnace power plants. Three-dimensional overhaul models in the field of combustion and power station boilers were developed during the past 15 years but 3D codes became ready for application in technical praxis only a several years ago, Ref. [2], still requiring the improvements in many aspects.

The main aim of numerical investigations performed for the purpose of the paper was to verify the computer code for simulation of turbulent flow in 3D geometry in the beginning of development. Provided we want to have a sound numerical basis for simulations of practical phenomena, our predictions of both mean (time averaged) and fluctuating turbulent flow field characteristics have to been successfully compared to the corresponding results of measurements. Simultaneously, the computer code must satisfy the convergence criterion as good as possible.

2. MATHEMATICAL MODEL

The Lagrangian statements of the fundamental laws of mechanics are cast into an Eulerian framework for use in fluid mechanics by using the Reynolds transport theorem, see Ref. [3]. In general index notation within *Eulerian flow field*:

$$\frac{\partial}{\partial x_j}(\rho U_j \Phi) - \frac{\partial}{\partial x_j}\left(\Gamma_\Phi \frac{\partial \Phi}{\partial x_j}\right) = S_\Phi \tag{1}$$

supposing that there is time averaged stationary flow and turbulent fluctuations. In Eqn. (1) Φ, Γ_Φ and S_Φ are general variable (time averaged), diffusion coefficient and source term, respectively.

Modeling equations in orthogonal Decartes coordinate system, for single-phase incompressible (ρ = const.) turbulent flow at isothermal conditions, in 3D - space:

- Continuity equation

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} = 0 \tag{2}$$

- Momentum equations

for: 'k' = 1 (x-direction, $x_1 = x$, $U_1 = U$), 'k' = 2 (y-direction, $x_2 = y$, $U_2 = V$), 'k' = 3 (z-direction, $x_3 = z$, $U_3 = W$)

$$\rho U \frac{\partial U_k}{\partial x} + \rho V \frac{\partial U_k}{\partial y} + \rho W \frac{\partial U_k}{\partial z} - \mu_{eff}\left(\frac{\partial^2 U_k}{\partial x^2} + \frac{\partial^2 U_k}{\partial y^2} + \frac{\partial^2 U_k}{\partial z^2}\right) = -\frac{\partial P}{\partial x_k} \tag{3}$$

-Transport equation for turbulence kinetic energy

$$\rho U \frac{\partial k}{\partial x} + \rho V \frac{\partial k}{\partial y} + \rho W \frac{\partial k}{\partial z} - \frac{\mu_{eff}}{\sigma_k}\left(\frac{\partial^2 k}{\partial x^2} + \frac{\partial^2 k}{\partial y^2} + \frac{\partial^2 k}{\partial z^2}\right) = G - C_D \rho \varepsilon \tag{4}$$

$$\begin{aligned} \boldsymbol{G} = {} & 2\mu_{eff}\left[\left(\frac{\partial U}{\partial x}\right)^2 + \left(\frac{\partial V}{\partial y}\right)^2 + \left(\frac{\partial W}{\partial z}\right)^2\right] + \\ & + \mu_{eff}\left\{\left[\frac{\partial V}{\partial x} + \frac{\partial U}{\partial y}\right]^2 + \left[\frac{\partial W}{\partial y} + \frac{\partial V}{\partial z}\right]^2 + \left[\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x}\right]^2\right\} \end{aligned} \tag{5}$$

-Transport equation for dissipation rate of turbulence kinetic energy

$$\rho U \frac{\partial \varepsilon}{\partial x} + \rho V \frac{\partial \varepsilon}{\partial y} + \rho W \frac{\partial \varepsilon}{\partial z} - \frac{\mu_{eff}}{\sigma_\varepsilon}\left(\frac{\partial^2 \varepsilon}{\partial x^2} + \frac{\partial^2 \varepsilon}{\partial y^2} + \frac{\partial^2 \varepsilon}{\partial z^2}\right) = \frac{\varepsilon}{k}(C_{\varepsilon_1}\boldsymbol{G} - C_{\varepsilon_2}\rho\varepsilon) \tag{6}$$

For closure of Reynolds differential equations, i.e. Eqn. (2)–Eqn. (3),(for modeling of turbulent stresses), concept of 'turbulence viscosity' μ_t is used, where $\mu_{eff} = \mu+\mu_t$ is 'effective viscosity' as a sum of laminar and turbulence viscosity.

For mathematical description of the turbulence viscosity, a standard two-equation *k-ε model of turbulence* has been used:

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \tag{7}$$

Constants C_μ , $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, C_D and Prandtl-Schmidt numbers for turbulence kinetic energy σ_k and its rate of dissipation σ_ε , used in the model are given in Table 1. Their values are in accordance with standard values from literature, except for σ_ε , which is usually 1,30 but here it has been calculated from:

$$C_{\varepsilon_1} = C_{\varepsilon_2} - \frac{\kappa^2}{\sigma_\varepsilon}\frac{1}{\sqrt{C_\mu}} \tag{8}$$

using Von-Karman's constant κ = 0,4187 obtained by numerical optimization.

Table 1. Constants of k-ε model of turbulence

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_D	σ_k	σ_ε
0,09	1,44	1,92	1,00	1,00	1,22

Of all the two-equation models, the k-ε model of turbulence has the widest application for confined turbulent flows, see Ref. [3]. It has been successfully tested in a number of different reacting and nonreacting flow environments and it is relatively simple, especially compared to the Reynolds stress turbulence models. The shortages include the assumption of the Boussinesq gradient-diffusion hypothesis and the assumed isotropy of the eddy diffusivity.

For pulverized coal systems without swirl, the k-ε model seems to be the most practical choice. Though, strongly swirling flows are of particular interest to combustion of pulverized coal. Such flows are characterized by a highly nonisotropic nature, especially within and in the vicinity of the recirculating zone. In reality, the region of the recirculation zone is characterized by large amount of turbulence kinetic energy generation due to the high local strain rates and gradients, which in turn is associated with a nonisotropic turbulence structure. The modification of the k-ε model, often proposed, includes the modifications of the source term coefficients in the dissipation equation through the Richardson number. Although this approach helps to alleviate a portion of the problem, it does not provide a complete solution to complex swirling flow field, introducing the additional complexity in the model. For these reasons, we have adopted the standard, unmodified k-ε model of turbulence.

Considering initial and boundary conditions, we have applied the usual approach for elliptical type of differential equations in modeling praxis. At inlet cross-section known flow conditions are set. Initialization for ε (the rate of dissipation of turbulence kinetic energy) has been done by use of a well known expression

$$\varepsilon_{IN} = \frac{k_{IN}^{\;1.5} C_{\mu}^{\;0.75}}{l_{\varepsilon}} \tag{9}$$

where l_{ε} - dissipation length scale is the scale of turbulence energy carrying vortices, estimated in the work in such a way to enable the best agreement between calculated values for k with the experimental results. At outlet section and at the plane of symmetry (in the case where the computer code considering only a half of the cubic box has been used) the gradients of all scalar quantities are set to be zero, while for axial velocity it is important to satisfy the condition of the continuity of the flow at outlet section. Near the walls of the calculation domain, logarithmic velocity profile and corresponding expressions for the friction stress (through the 'wall functions') have been prescribed.

For deriving of corresponding finite-difference equations, the control volume procedure has been used, within the framework of the so-called staggered numerical grid, including the hybrid numerical scheme and the SIMPLE calculation algorithm, Ref. [4]. For solving of the obtained system of algebraic equations, the SIPSOL procedure, see Ref. [5], cast into the 3D form, has been used. Stabilization of the iteration process is performed by means of subrelaxation technique. We have successfully applied two numerical grids, but with equal dimensions of the corresponding control volumes: grid with $22 \times 12 \times 22$ nodes, considering a half of the cubic box, using the fact that there is x-z plane of symmetry going through both inlet and outlet windows of the box, as well as the grid with $22 \times 22 \times 22$ nodes, stretching over the whole space of the cubic box. Uniform numerical grid has been applied in both cases. It has been set that the convergence criterion of the computer code is satisfied when the value of maximum of the normalized residuals for mass and velocity components in all three directions becomes less than prescribed value of 10^{-4}.

RESULTS OF MODELING AND DISCUSSION

Time averaged flow field – comparisons to experiments

As a referent case for computer code verification, we have chosen a water flow through the cubic box, sides 50 cm, with inlet and outlet square windows, sides 15 cm. The coordinate axes are oriented according to Fig. 1. Flow visualizations had been made by taking pictures by means of plane light beams and measurements had been made by Laser-Doppler anemometry. Comparisons of the predictions and measurements were performed for the vertical plane going through the centers of both inlet and outlet windows, which was also the symmetry plane of the cubic box. The inlet window starts from the location y = 17,5 cm; z = 30 cm while the outlet one starts at y = 17,5 cm; z = 5 cm from the referent point of the coordinate system.

Although the cubic box is of a relatively simple geometry, it is interesting for it differs from usually considered cases where dimension in one direction is a dominant one. Additionally, it is not easy to find in literature referent experimental data considering 3D configuration obtained not only for time averaged flow field, but for turbulence characteristics, such as turbulence kinetic energy, as well. Results of experiments have been taken from Ref. [6], where the results of numerical simulation, performed by means of both k-ε turbulence model and LES - 'Large Eddy Simulation' model are also presented.

The calculations have been performed here for the whole space of the cubic box and also for the half of it, taking into account the fact that there is x-z plane of symmetry at y = 25 cm, and by using the control volumes with the same dimensions in both cases.

A turbulent water flow with time averaged velocity U_{IN} = 0,24 m/s (constant, flat profile over the inlet section) enters the domain through the square window. Reynolds number with respect to the window side Re = 36000. The flow impinges the opposite wall, recirculates and progressively moves towards the exit square window in the lower half of the box. Predictions are not given for the plane of symmetry itself, but as close to it as possible. U and W velocities and turbulence kinetic energy were calculated for y – coordinate that corresponds to the numerical nodes (i, j=2, k). This means that the values were calculated and given for the plane at a location y = 1,25 cm, i. e. very close to the symmetry plane.

In the case of the whole cube geometry, results showed acceptable symmetry in y – direction. When symmetry in a flow field exists, we have the opportunity either to save the computation time considerably, applying numerical grid with fewer nodes, or to try to attain better accuracy, keeping the original grid refinement, but for the half of the calculation domain. For results presented, we have used the latter approach. In addition, the computer program has shown by no doubt a good convergence.

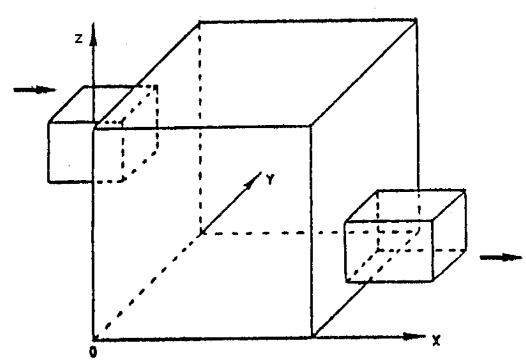

Fig. 1. Geometry of the cubic box with inlet and outlet windows shifted along the z-direction

A comparison between numerical results and the experimental ones, considering mean, i.e. time averaged velocity vector field in the symmetry plane x-z is quite satisfactory, illustrated by Figs. 2. and 3. When compared to the computations presented in Ref. [6], performed by means of the 3D, but standard k-ε model of turbulence, similar to the model used in this paper, calculations shown in Fig. 3. agree even better with measurements, which means reflect the physicality of the flow better.

It should be emphasized that Ref. [6] gives actually the results of solving time dependent, i.e. non-stationary Navier-Stokes equations in three dimensions. Some results of computations in Ref. [6] could be understood as an initial case of a general, non-stationary flow, so being appropriate for comparison to the results of calculations of a stationary time averaged flow, considered in our paper.

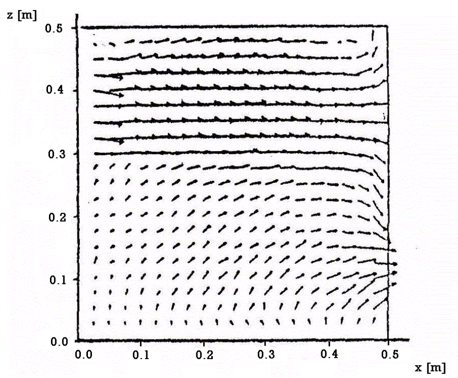

Fig. 2. Measured mean velocity vectors in a symmetry plane of the cubic box through the centers of both inlet and outlet windows

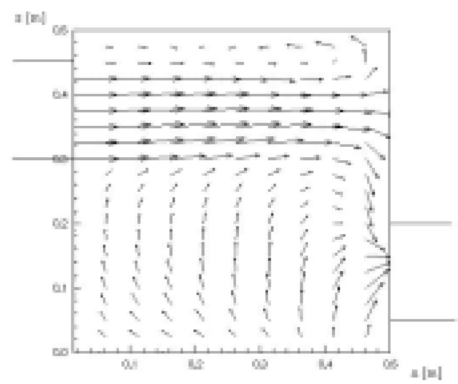

Fig. 3. Predicted mean velocity vectors in a symmetry plane of the cubic box through the centers of both inlet and outlet windows

Time averaged flow field – considerations on physicality

In Fig. 3. two different recirculating zones are shown, including a very intensive vorticity in the upper right corner. Both inflow and outflow of the fluid can be noticed quite clearly. For getting more complete picture of the flow field, it is also useful to consider streamlines in different planes. In these figures, x - coordinate does not start from zero, but from the distance which is, in fact, x -coordinate of the grid node from which the calculation of the U - velocity begins in the computer program and that is the third node of the grid staggered in the negative direction of x - axis. If the flow is 2D, Fig. 3. would give a complete information on the flow field. If we could suppose the infinite dimension in y - direction, it would be the case of the plane symmetric 2D flow. But 3D flow is considered here, where the influence of the flow domain boundaries, i.e. walls could not be neglected in any direction. It is very important to point this out, because the real flows in technical systems have a 3D character. Someone who is used to considering 2D flows and with the argument that the plane of symmetry is the representative one also in 3D geometry, might not expect to find out anything essentially new, if the streamlines in the other planes are given as well. Figs. 4., 5., 6. and 7. solve this dilemma. The flow field in a half of the box is shown.

Figures 4. and 5. lead to conclusion that the vortices are placed where it could be expected, i.e. in the regions of so called 'hydrodynamic pockets' with both inflow and outflow streams simulated correctly. It is also interesting to note the simplification of the flow field picture downstream, observed in y-z planes, Figs. 6. and 7., with the reduction of the complex flow at inlet to only one large vortex near the outlet.

As it has been shown, a 3D flow picture is tremendously complex. If we want to 'visualize' the whole flow field numerically, we should present the streamlines in a number of planes, perpendicular to all of three coordinate axes. Cube geometry, although relatively simple, emphasizes a three-dimensionality problem perhaps the most obviously, because in this case it is completely unjustified to neglect the influence of the boundaries – walls in any direction. Also, the conclusion is that even a simple geometry imposes a necessity of problem consideration in all of the three dimensions.

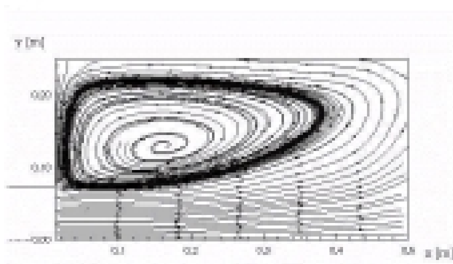

Fig. 4. Predicted streamlines in x-y plane crossing the center of the inlet opening

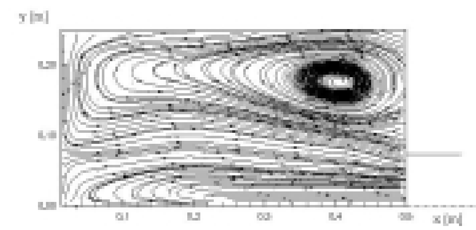

Fig. 5. Predicted streamlines in x-y plane crossing the center of the outlet opening

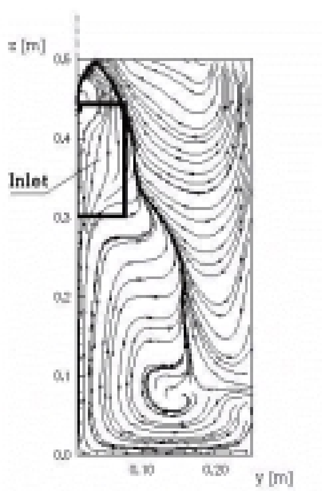

Fig. 6. Predicted streamlines in y-z plane at a distance of 8,75 cm from inlet opening

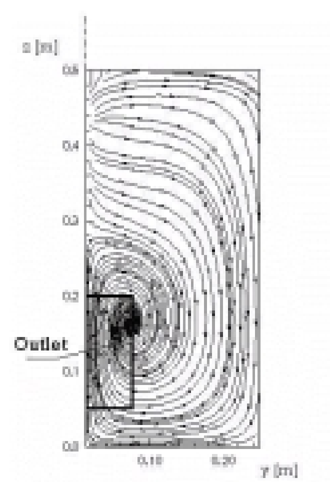

Fig. 7. Predicted streamlines in y-z plane at a distance of 11,25 cm from outlet opening

Turbulence fluctuations – comparisons to experiments

Speaking of the fluctuating flow field, turbulence kinetic energy could be considered a measure of the intensity of the turbulence fluctuations in the three directions. A standard k-ε model of turbulence extended to a 3D flow has been used in this paper. The initial profile for turbulence kinetic energy is in accordance with the measured profile for the cross-section over the entire cubic box and near the inlet, at a distance $x = 5$ cm. Predictions for turbulence kinetic energy have been compared to the corresponding experimental results, taking from Ref. [6]. Comparisons are given for the same x-z plane as for time averaged flow field and at different axial positions, Fig. 8. Generally, the agreement of calculations performed for the purpose of this work with referent measurements is good. Agreement of our calculations with experiments is similar or better compared to predictions from Ref. [6].

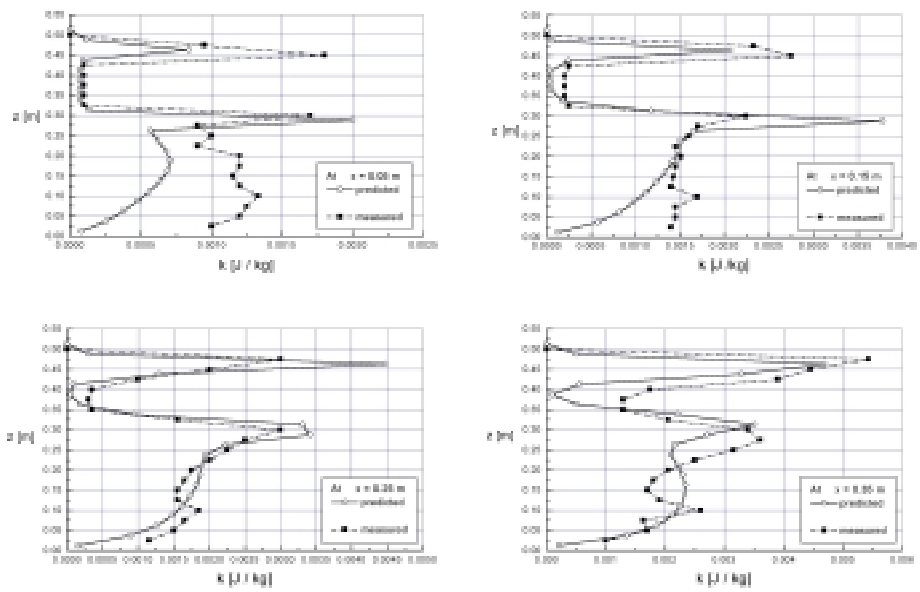

Fig. 8. Downstream change of turbulence kinetic energy in x-z symmetry plane of the cubic box

4. Conclusion

In the paper, the equations, assumptions and results of a 3D mathematical model, using the two - equation k-ε approach, for incompressible turbulent single-phase flow in the cubic box are presented. When compared to the corresponding experimental results for both time averaged flow field and turbulence kinetic energy, predictions performed for the purpose of this work have shown a good agreement. Conclusions, based on the calculation results analysis, could be presented as follows:

- basic mathematical model and computer code developed for the calculation of a three-dimensional single-phase isothermal turbulent flow have been confirmed, with respect to a time averaged flow field and turbulence kinetic energy as well,

- a computer program derivative which gives the opportunity of using finer numerical grid has been developed, considering the existence of the plane of symmetry and providing a good convergence of the solutions,
- it has been shown that even a relatively simple, but 3D geometry, gives a very complex flow field, imposing the application of 3D models, i.e. a real three-dimensional space computations, whenever it is important to obtain a detailed information on the flow field.

Numerical predictions presented in the paper have been performed as a starting phase in development of a complex 3D mathematical model of turbulent flow, with possible application in simulation of process engineering equipment and power plants, such as pulverized coal furnaces.

REFERENCES

1. J. M. Jones, M. Pourkashanian, A. Williams, R. K. Chakraborty, J. Sykes, Laurence D.: *Modelling of Coal Combustion Processes - A Review of Present Status and Future Needs*, Fifteenth Annual International Pittsburgh Coal Conference, Pittsburgh, U.S.A., September, 1998.
2. L. Douglas Smoot: *A Decade of Combustion Research*, Prog. Energy Combust. Sci., Vol. 23, No. 3, 1997, pp. 203-232.
3. L. Douglas Smoot, Philip J. Smith: *Coal Combustion and Gasification*, Plenum Press, New York, U.S.A., 1985.
4. S. V. Patankar: *Numerical Heat Transfer and Fluid Flow*, Hemisphere, New York, U.S.A., 1980.
5. M. Peric, G. Scheuerer: *Cast - A Finite Volume Method for Predicting Two-dimensional Flow and Heat Transfer Phenomena*, GRS - Technische Notiz SRR-89-01, Garching, Deutschland, September, 1989.
6. F. Baron, D. Laurence: *Large Eddy Simulations of a Wall-Bounded Jet Flow and of Homogeneous Shear Flow*, Proceedings of Fourth Symposium on Turbulent Shear Flows, September 12-14, 1983, Karlsruhe, F.R.Germany, pp. 4.7 - 4.12.

MATEMATIČKO MODELIRANJE TRODIMENZIONALNOG IZOTERMNOG MONOFAZNOG TURBULENTNOG STRUJANJA U GEOMETRIJI OBLIKA KOCKE

Simeon Oka, Srdjan Belošević

Numerička istraživanja, opisana u ovom radu, izvedena su kao početna faza u razvoju kompleksnog trodimenzionalnog matematičkog modela, koji bi trebalo da nađe primenu u simulaciji procesa u ložištima za ugljeni prah. Razvoj matematičkog modela za realne trodimenzionalne geometrije je veoma poželjan ako hoćemo da steknemo svu veštinu i iskustvo potrebno za modeliranje složenih strujanja u tehničkoj praksi postrojenja procesne tehnike, termotehničke opreme i elektrana.

*Turbulentno strujanje nekompresibilnog fluida kroz geometriju oblika kocke pri izotermnim uslovima, opisano je sistemom po vremenu osrednjenih jednačina održanja, uz primenu dvojednačinskog **k-ε** modela turbulencije i **SIMPLE** proračunskog algoritma. Za izvođenje odgovarajućih diferentnih jednačina, primenjena je metoda kontrolnih zapremina. Rezultati proračuna upoređeni su sa rezultatima merenja uzetim iz literature. Data je i analiza numerički dobijenog strujnog polja sa stanovišta fizikalnosti.*

Turbulentni mlaz vode ulazi u oblast strujanja (kocka sa stranama dužine 50 santimetara) kroz kvadratni otvor (sa stranicama od 15 santimetara). Mlaz udara u naspramni zid i delom se kreće

recirkulaciono. Pomera se prema izlaznom kvadratnom otvoru (sa stranicama od 15 santimetara) u donjoj polovini kocke. Vizuelizacija strujanja bila je izvedena fotografisanjem pomoću ravanskih svetlosnih zraka, a merenja su izvršena Laser-Dopler anemometrijom.

Poređenja rezultata su izvedena u vertikalnoj ravni koja ide kroz centar i ulaznog i izlaznog otvora. Vektori srednje brzine, dobijeni numerički, zadovoljavajuće se slažu sa onima dobijenim merenjem. Pored toga, prikazane su strujnice u različitim ravnima, ističući složenost trodimenzionalnog strujnog polja, čak i za relativno jednostavnu geometriju. Geometrija oblika kocke je interesantna i zato što se razlikuje od slučajeva koji se obično razmatraju, a u kojima je dimenzija u jednom pravcu dominantna. Proračunate vrednosti kinetičke energije turbulencije, date za različite aksijalne pozicije, dovoljno dobro se slažu sa izmerenim.