ANNALS OF FACULTY ENGINEERING HUNEDOARA
– INTERNATIONAL JOURNAL OF ENGINEERING
Tome X (Year 2012) – FASCICULE 3 (ISSN 1584 – 2673)

[1.] Anna LECHEVA, [2.] Ivanka ZHELEVA

NON-UNIFORM GRID CONSTRUCTION FOR NUMERICAL SOLVING OF NAVIER-STOCKES EQUATIONS FOR HYDRODYNAMIC INVESTIGATION OF A CHEMICAL REACTOR WITH A MIXER

[1.] DEPARTMENT OF MATHEMATICAL ANALYSIS, UNIVERSITY OF RUSE, BULGARIA
[2.] DEPARTMENT OF THERMO HYDRO-AND PHNEUMO TECHNIQUES, UNIVERSITY OF RUSE, BULGARIA

ABSTRACT: *Non-uniform grid construction for numerical solving of Navier-Stokes equations is described in the present paper. The Navie-Stokes equations which describe hydrodynamics in the chemical reactor with a mixer are approximated with second order of accuracy finite differences. The geometrical area is very complex because of convex mixer corners in the flow. Finite-difference grid is constructing via adding points near the solid boundaries of the domain, where the gradients of the velocity are high. Computational tests with two and three added points are provided. The geometrical area and the numerical results are graphically presented.*
KEYWORDS: *Navier-Stokes equations, non-uniform grid, convex corners in the flow, cylindrical reactor with a mixer, hydrodynamics, Reynolds number*

INTRODUCTION

The mechanical mixing is one of the most energy consuming operations in the chemical industry and biotechnology. Studying the hydrodynamics of fluids in chemical reactors and bioreactors with mechanical mixing caused the interest of researchers since the mid-fifties of the last century. The first researches in this area were conducted in small experimental laboratory glass containers with transparent walls and the main conclusions were made by direct observations and measurements of the velocity field [1]. One of the pioneers in this area is the Japanese scientist Nagata. He studied the problems of mixing of pure engineering point of view and summarize the results in sensational for its time book "Mixing: Principles and Applications" in 1975. The rapid hydrodynamic studying of the fluid motions in reactors with mixing was begun in the early eighties of last century, when the computer technology became increasingly developed. Theoretical models were created and computational experiments were conducted in parallel compared with direct observations and laboratory experiments.

In recent years, most researchers who conducted computer simulations use the CFD (Computational Fluid Dynamics) software packages. Using such software requires large computational resources. Usually the calculations continue about 1000 CPU time with Sun SPARC workstation [2]. The obtained numerical results are compared with results from laboratory experiments conducted in parallel. There are many modern ways to experimentally determine the velocity field. Some of them are: determining of the velocity field by visualizing particles injected into the fluid - particle imaging velocimetry (PIV) [1,2], determining of the velocity field by laser - Doppler system velocimetry [1,2,3], defining the velocity field by injecting different fluorescent dyes in the fluid - dye injection photographs [1], est. In all these systems, the laboratory results are saved by laser plaques or digital cameras in a short period of time (about 1-15 ms.). Then results are interpolated and fluid velocity is obtained throughout the volume of the laboratory container.

Nevertheless, this engineering approach is not actually sufficient for complete investigation of fluid motion in the reactor. The construction of proper mathematical models and numerical investigation of hydrodynamics in such reactors with mixing via computer simulations eliminate the need of expensive reproduction of the processes in the laboratory and gives complete data of the fluid behavior.

MATHEMATICAL MODEL

The construction of mathematical model includes description of geometrical area, the main equations which describe the fluid motion and the boundary and initial conditions for all unknown functions.

Geometrical area

To construct a mathematical model for studying the process of hydrodynamics we assume that the reactor is a cylindrical vessel with a flat bottom with a given radius and height. The reactor is filled

with reaction mixture, which can be assumed that it is homogeneous or inhomogeneous fluid, depending on the technology. The mixer is located on the shaft axis of the cylinder and rotates with constant set angular velocity. The fluid motion in the reactor is caused by the rotation of the shaft with a mixer stirring the objective of homogenization of the fluid or intensification of the processes.

Studying of hydrodynamics in the reactor with mechanical mixing, we keep the hierarchy of models, starting from simpler to more complex model. In this sense, the reactor is a right circular cylindrical container with a given radius R and height Z. For reasons of convenience, we introduce the cylindrical coordinate system (r,φ,z)*, which is shown in Figure 1. The reactor is filled with reaction mixture. We assume that it is a viscous incompressible Newtonian fluid and carried axis-symmetric rotating. The disk has given radius R1 and thickness L1. It is placed at H1 height from the bottom and it is rotating with the constant angular velocity* Ω *(Figure 1).*

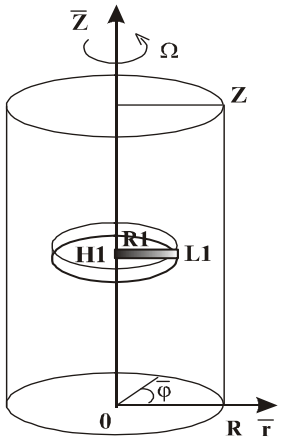


Figure 1. Scheme of the reactor with a disc

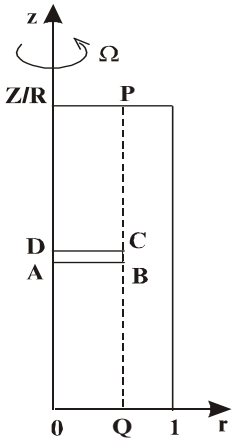


Figure 2. Scheme of the computational area

It is necessary to have a geometric and dynamic similarity between the studying reactors. Linear characteristic dimensionless parameter is introduced to construct an adequate mathematical model. In present investigation we choose the cylinder radius R to be the characteristic linear dimension. Therefore, all geometric parameters become dimensionless through the following equalities:

$$r=\frac{\bar{r}}{R},\ z=\frac{\bar{z}}{R},\ R1=\frac{\overline{R1}}{R},\ L1=\frac{\overline{L1}}{R},\ H1=\frac{\overline{H1}}{R},\ H2=\frac{\overline{H2}}{R},\ H3=\frac{\overline{H3}}{R}. \tag{1}$$

After using (1), the cylindrical coordinate system becomes (r, φ, z). We do some more simplifying assumptions - as the reactor is a cylindrical vessel and the mixer is a disk that is attached to the cylinder axis then the geometric area has symmetry about any plane through the axis of symmetry of the cylinder. Therefore, the movement of the fluid in the reactor can be assumed as axis symmetrical. Then, due to axial symmetry of the flow, we assume that the unknown functions that describe the fluid motion depend only on r and z. In this case we can consider only the half of the axial section of the cylinder. Thus the three-dimensional (3D) geometric area in Figure 1 can be reduced to 2D "computational" geometric area on Figure 2.

Thus for the variables r and z we have $0 \le r \le 1$ *and* $0 \le z \le Z/R$.

Basic equations

The equations which describe the motion of viscous fluids [5, 6] are written on the base of the fundamental laws of conservation in Continuum Mechanics. We examine the flow in the reactor long enough after the mixing process start and we look for a steady solution. Therefore, we can assume that the unknown functions do not depend on time also [7].

We introduce the stream function ψ*, the vorticity of the velocity* ω *and the momentum of the tangential velocity M. The basic equations can be written in dimensionless form in terms of the introduced functions as follows:*

$$\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial\psi}{\partial r}\right)+\frac{\partial}{\partial z}\left(\frac{1}{r}\frac{\partial\psi}{\partial z}\right)=-\omega \tag{2}$$

$$\frac{1}{r}\frac{\partial rUM}{\partial r}+\frac{\partial WM}{\partial z}=\frac{1}{\mathrm{Re}}\left[r\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial M}{\partial r}\right)+\frac{\partial^2 M}{\partial z^2}\right], \tag{3}$$

$$\frac{\partial U\omega}{\partial r}+\frac{\partial W\omega}{\partial z}-\frac{1}{r^3}\frac{\partial M^2}{\partial z}=\frac{1}{\mathrm{Re}}\left[\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial r\omega}{\partial r}\right)+\frac{\partial^2\omega}{\partial z^2}\right]. \tag{4}$$

The relationship between the first U and third W component of the velocity vector $\vec{V}$ *(U, V, W) and the stream function* ψ *in cylindrical coordinate system is the s following:*

$$U=-\frac{1}{r}\frac{\partial\psi}{\partial z},\qquad W=\frac{1}{r}\frac{\partial\psi}{\partial r}. \tag{5}$$

In equations (2) – (5), $\mathrm{Re}=\frac{\Omega R^2}{\nu}$ *is the Reynolds number,* $\vec{\omega}=rot\vec{V}=(0,\omega,0)$ *is the vorticity vector of the velocity and M = Vr is the magnitude of the momentum of tangential velocity in dimensionless form.*

We have five equations (2) – (5) with five unknown functions - the stream function ψ, the vorticity of the velocity ω, the momentum of the tangential velocity M and the first U and third W component of the velocity vector.

These equations describe the present mathematical model.

Boundary conditions

It is well known that the different fluid motions, i.e. different solutions of the Navier-Stokes equations differ from each other because of its boundary and initial conditions as well as some dynamic parameters of flows, such as the Reynolds number Re [4, 5, 6]. This determines the important role of correct statement of boundary conditions for all specific hydrodynamic problems.

We examine the flow of the fluid in area with moving and non-moving solid boundaries. Traditional boundary conditions are adhesion and "no-slip" conditions of viscous fluid on the solid non-moving walls of the reactor, i.e. zero boundary conditions for all components of the velocity vector $\vec{V} = 0$. The velocity of the fluid coincides with the linear velocity of the stirrer Ωr on the rotating disk.

All solid boundaries of the area, the walls of the disc and the line of symmetry are isolines of the stream function. Therefore, the boundary conditions for the stream function are:

$$\psi = 0 \quad and \quad \frac{\partial \psi}{\partial n} = 0, \tag{6}$$

where n is the normal unit vector to the boundary lines [6].

Thus formulated problem for Navier - Stokes equations solving is open, since there are two boundary conditions for the stream function and there is no physical boundary condition [6]for the vorticity. This leads to considerable difficulties in the system solving if the equations are treated separately. Therefore, we set mathematical boundary conditions for the vorticity, which are calculated from the values of the stream function near the boundaries [8]. This explains the necessity of simultaneous solving of the equations (2) and (4).

The boundary conditions for the first U and third W components of the velocity vector, for the stream function ψ and the magnitude of the momentum of tangential velocity M are given in details in Table 1 (Fig.1, Fig.2).

Table 1. Boundary conditions for U, W, ψ, M

boundary	coordinates	first component U of the velocity	third component W of the velocity	stream function ψ	momentum M
bottom	$z = 0$ $0 \le r \le 1$	$U = 0$	$W = 0$	$\psi = 0$	$M = 0$
top	$z = Z/R$ $0 \le r \le 1$	$U = 0$	$W = 0$	$\psi = 0$	$M = 0$
wall	$r = 1$ $0 \le z \le Z/R$	$U = 0$	$W = 0$	$\psi = 0$	$M = 0$
line of symmetry	$r = 0$ $0 \le z \le Z/R$	$U = 0$	$W = 0$	$\psi = 0$	$M = 0$
bottom wall AB of the disc	$z = H1/R$ $0 \le r \le R1/R$	$U = 0$	$W = 0$	$\psi = 0$	$M = r^2 / R^2$
top wall CD of the disc	$z = (H1+L1)/R$ $0 \le r \le R1/R$	$U = 0$	$W = 0$	$\psi = 0$	$M = r^2 / R^2$
vertical wall BC of the disc	$r = R1/R$ $H1/R \le z \le (H1+L1)/R$	$U = 0$	$W = 0$	$\psi = 0$	$M = r^2 / R^2$

FINITE-DIFFERENCE GRID CONSTRUCTION

It is known that for many hydrodynamic problems an analytical mathematical solution can be found not always. In such a case the model system could be solved numerically [1, 2, 3, 4, 5, 6]. The numerical solutions are "close" to the exact solution and differ from it with a given accuracy which depends on the used numerical algorithm.

To implement some numerical algorithms for system of partial differential equations solving, first of all this system should be transformed to a finite-difference analogue. For this purpose it is necessary to replace the continuous arguments variation area by an area of discrete variation of the arguments, i.e. to construct a finite-difference grid and after that all PDF equations to be transformed into algebraic difference equations [7].

We use finite differences of second order accuracy to approximate the system.

The computational area shown in Figure 2 is very complex because of the convex corners of the disc ABCD.

The velocity gradients near the boundaries are significant [5, 6, 7]. This is because of the rapid reduction of the fluid velocity to zero on the solid non moving boundaries, where the conditions for

adhesion it satisfied. There are significant changes of velocity in a small area near the boundary, which increases the size of viscous terms in the Navier-Stokes equations. Using of an uniform grid in these areas is not appropriate, as such a grid has to be with very small steps in both directions r and z because of the velocity large gradients there. If the steps are very small that would lead to difficult and slow computational process. This approach takes more CPU time and memory, and risk of quantitative calculation errors in critical areas.

This disadvantage is overcome by constructing of a grid with irregular thickening in areas with large solution gradients. These large gradients are expected to be around the wall, bottom and top of the reactor and near the rotating disc, i.e. around the solid boundaries of the area where the fluid satisfies the adhesion boundary conditions.

The non-uniform grid

Partly uniform grid consisting of rectangular meshes is constructed initially in the geometric area on Figure 2. The steps of this initial grid are h_r in r direction and h_z in z direction. Points A, B, C, D, P, Q on Figure 2 are nodes of the grid. This initial grid is shown in Figure 3, where $h_r \neq h_z$. If $h_r = h_z$ then the initial grid is uniform with square cells.

Parameters Hbr, Hbz and Hbl are computing parameters, which describe the dimensions of the disc ABCD on Figure 2. Parameter Hbr describes the radius of the disk. Parameter Hbz and respectively Hbl describe the height of the disc place from the bottom of the reactor and its thickness. Thus, the bottom corner of the disk B is denoted by (Hbr, Hbz), and the upper corner of the disk C is denoted by (Hbr, Hbz + Hbl).

Then, each interval of the initial grid, which is neighboring to some of the solid boundaries of the area, is divided into two equal subintervals with step $h_r/2$ in r direction and $h_z/2$ in z direction. After that, each subinterval, which is neighboring to the solid boundaries of the area, again is divided into two equal subintervals with steps accordingly $h_r/4$ and $h_z/4$, etc.

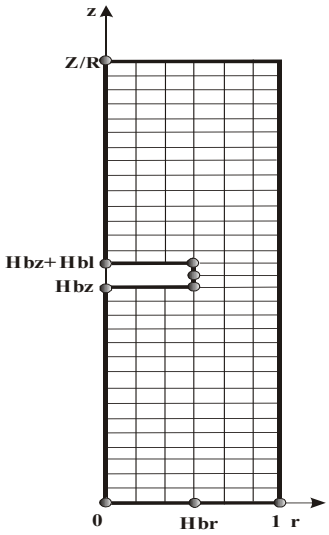


Figure 3. Initial uniform grid

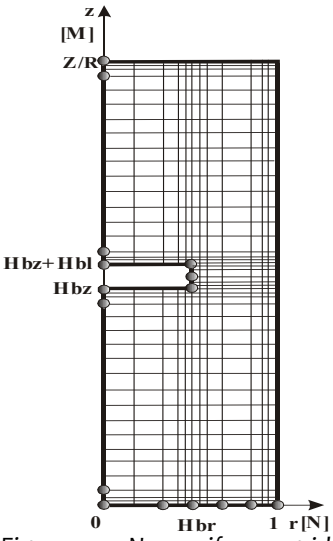


Figure 4. Non-uniform grid with n = 2 added points

All intervals of the initial grid, which are neighboring to the lower corner (Hbr, Hbz) and the upper corner (Hbr, Hbz + Hbl) of the disc is divided equally in both directions r and z. Thus, the grid has received irregular thickening around the convex corners of the disc.

We denote by n the number of points added in any interval of the initial grid in its division of the subintervals. The number of points added in all intervals is equal for all border areas. When n = 0, obviously, in computational geometry area we have the initial grid. For example, if n = 2, then the number of points added in the direction r is 3n, because we have two points added near the vertical wall of the cylinder, two points added on the right side of the vertical wall BC of the disc and two points added on the left side of the vertical wall BC of the disc. The number of points added in the z direction is 6n, because we have two points added to the bottom boundary of the area, two points added to the top boundary of the area, two points added above and below the lower wall AB of the disc, and two points added above and below the upper wall CD of the disc. Around the axis of the cylinder is not thickening of the grid, because there is no solid boundary and therefore no condition of adhesion of the fluid. Conditions for symmetry are set there [6].

Finally we denote by N the number of all points in r direction, respectively, with M the number of all points in the z direction of the resulting non-uniform grid. So, this non-uniform grid constructed with n = 2 added points is shown on Figure 4.

The constructed grid can be modified as the number n of added points increases in critical areas - near the disc and near the reactor walls.

NUMERICAL TESTS AND RESULTS

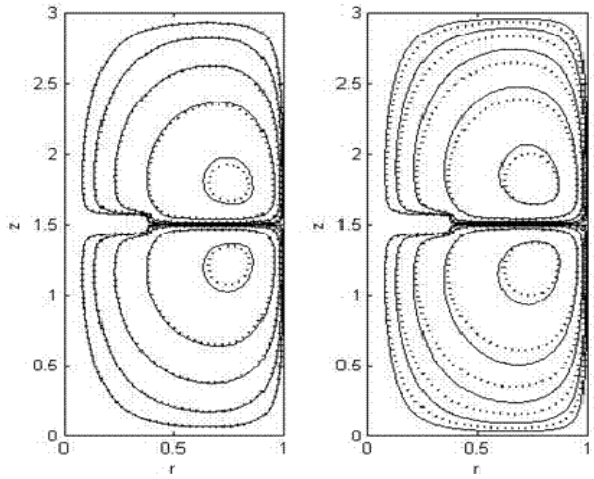
Numerical tests with n = 2 and n = 3 added points in critical areas near solid boundaries are provided. The Reynolds number Re is chosen to be Re = 1000. Cases with different steps of the initial uniform grid are examined: $h_r = h_z = 1/32$ and $h_r = h_z = 1/64$. The isolines of stream function are obtained and graphically presented in all cases on Figure 5.a,b and Figure 6.a,b.

Values of stream function isolines for all four cases are: ±0,00015096; ±0,00041035; ±0,0011154; ±0030321; ±0,008242. The positive values of stream function are observed in lower vortex fluid structure

and the negative values are observed in upper vortex fluid structure. There is symmetry with respect to the disk level between both structures in all four cases. We denote by (r_{max},z_{max}) the center of lower vortex fluid structure and by (r_{min}, z_{min}) the center of upper vortex fluid structure.

Table 2. Coordinates of fluid vortex structure

	1/32				1/64			
	r_{max}	r_{min}	z_{max}	z_{min}	r_{max}	r_{min}	z_{max}	z_{min}
2 points added	0.75	0.75	1.21875	1.78125	0.765625	0.76563	1.21875	1.78125
3 points added	0.78125	0.78125	1.21875	1.78125	0.765625	0.76563	1.1875	1.8125

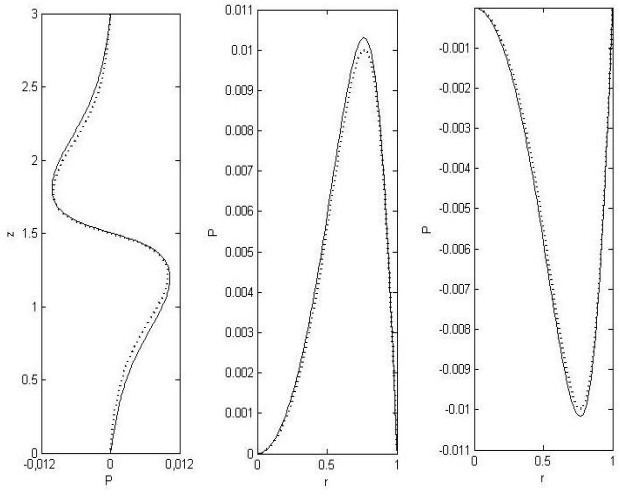


a *b*

Figure 5. Isolines of stream function. a) 2 points added for results with grid steps 1/32 and 1/64; b) 3 points added for results with grid steps 1/32 and 1/64

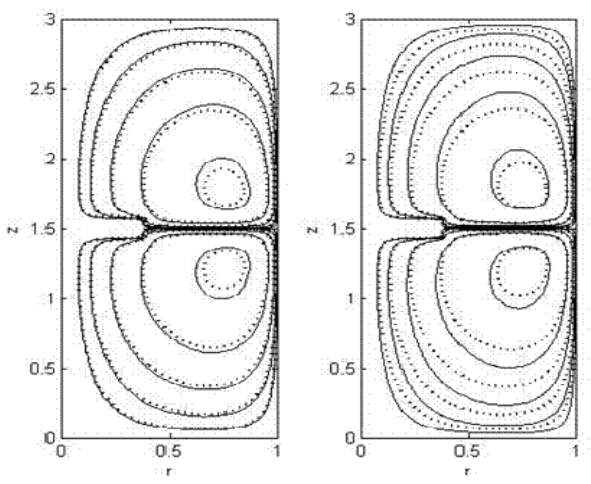
There is a displacement of centers of vortex fluid structures in r direction when the step of initial uniform grid is 1/32 and in z direction when the step of initial uniform grid is 1/64. This fact is due to the reduction of grid steps by half and, therefore, the refining of the non-uniform grid.

Sections through the vortex fluid centers for the result with grid step 1/32 and 1/64 with 2 added points are shown on Figure 7. These sections are made on level r = 0.75 in r direction (Figure7a) and z = 1.21875 for lower structure (Figure7b), respectively, z = 1.78125 for upper structure (Figure7c) in z direction.



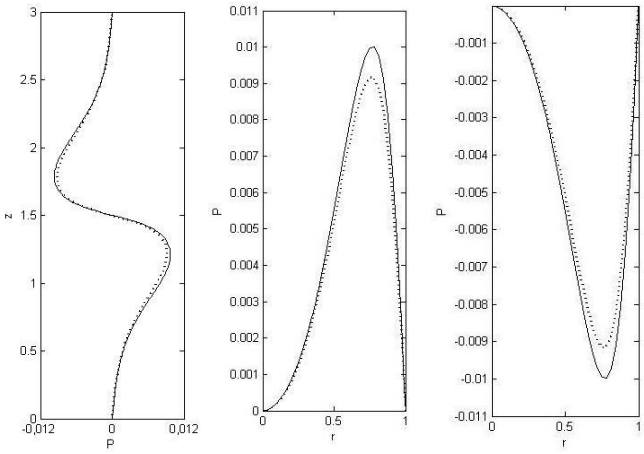
a *b* *c*

Figure 8. Sections through the centers of vortex fluid structures 1/32 and 1/64 – 3 points added



a *b*

Figure 6. Isolines of stream function a) 2 and 3 points added for results with grid steps 1/32; b) 2 and 3 points added for results with grid steps 1/64



a *b* *c*

Figure 7. Sections through the centers of vortex fluid structures 1/32 and 1/64 – 2 points added

Sections through the vortex fluid centers for the result with grid step 1/32 and 1/64 with 3 added points are shown on Figure 8. These sections are made on level r = 0.78125 in r direction (Figure8a) and z = 1.21875 for lower structure (Figure8b), respectively, z = 1.78125 for upper structure (Figure8c) in z direction.

Table 3 . Difference in percents

	2 points added (Figure 7)	3 points added (Figure 8)
$\psi_{positive}$	5.52%	2.63%
$\psi_{negative}$	5.38%	1.61%

We denote by solid line the result with grid step 1/32 and with point line the result with grid step 1/64, respectively.

Differences between these results are given in percents in Table 3. The maximum value of these differences is calculated in follow norm:

$$\psi_{positive(negative)} = \left| \frac{\psi_{1/64} - \psi_{1/32}}{\psi_{1/64}} \right| \%.$$

Obviously, from Table 3 follows that the best results are obtained when the grid steps of the initial uniform grid are $h_r = h_z = 1/64$ and $n = 3$ added points in boundary areas.

CONCLUSIONS

Mathematical model for investigation of fluid dynamics in cylindrical tank reactor with mechanical mixing is described. The Navie-Stokes equations are approximated with second order of accuracy finite differences. Non-uniform grid construction for numerical solving of these equations is provided via adding points near the solid boundaries of the domain, where the gradients of the velocity are high. Computational tests with two and three added points are made. The geometrical area and the numerical results are graphically presented.

The increasing of number of points near solid boundaries of the domain does not lead to significant increasing of CPU calculation time. There is a good agreement between the scheme accuracy and the available computing resources.

REFERENCES

[1.] *Fountain G. O., Kharhar D.V., Mezic I. and Ottino J. M., Chaotic mixing in a bounded three-dimensional flow, J. Fluid Mech., 2000, vol.417, pp. 265-301*

[2.] *Lamberto D. J., Alvarez M. M. and Muzzio F. J., Experimental and computational investigation of the laminar flow structure in a stirred tank, Elsevier Science Ltd., 1999, Chem. Ing. Sci. 54, pp. 919-142*

[3.] *Zalc J.M., Szalai E.S., Alvarez M.M. and Muzzio F.J., Using CFD to understand chaotic mixing in laminar stirred tanks, AIChE Journal, 2002, vol.48., No. 10, pp. 2124-2134*

[4.] *Bakker A., Hydrodynamics of stirred gas-liquid dispersions, PhD Thesis, 1992, Delft University of Technology, The Netherlands*

[5.] *Foias C., Manley O., Rosa R. and Temam R., Navier-Stokes Equation and turbulence, Cambridge University Press, UK, 2001*

[6.] *Roache P., Computation fluid dynamics, Hermosa Publishers, Albuquerque, 1976*

[7.] *Samarskii A., Introduction to theory of difference schemes, Nauka, Moscow, 1971, (in Russian)*

[8.] *Lecheva A., Boundary conditions for nonzero component of the vorticity vector in hydrodynamic problems with convex corners in the flow, Scientific works, University of Ruse, 2004, vol.41, issue 7.2, pp. 176-183 (in Bulgarian)*

[9.] *Zheleva I., Lecheva A., An algorithm for numerical investigation of viscous swirling flow in tank reactor with a mixer, Scientific works of University of Ruse, 2002, vol. 39, issue 2.2, pp. 128-133 (in Bulgarian)*

ANNALS OF FACULTY ENGINEERING HUNEDOARA
– INTERNATIONAL JOURNAL OF ENGINEERING