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3D-CALCULATION OF A VERTICAL SETTLER ON THE BASIS OF CFD-MODEL

The paper considers construction of a numerical model of mass transfer in a vertical settler. Modeling is based on the three-dimensional equation of the pollutant transfer model and the potential flow model. For numerical integration implicit difference schemes are used. The results of computational experiment are presented.

Key words: *numerical modeling, vertical settler, sedimentation, computational experiment, difference schemes.*

Introduction

At present, theoretical methods for calculation of vertical settlers are being actively developed in the world. It is related to the fact that experimental studies in this field require much time for the experiment organization, its realization and the experimental data processing. Besides, for the experimental research expensive equipment is used and the parameters of interest are measured without "introduction" of the device into the flow [1] (e. g. ADV system – *Acoustic Doppler Velocity measurements,* etc.), which not all laboratories can afford. In this regard, physical experiment cannot be a tool for everyday solutions to the problems that arise during the stage of designing structures or their reconstruction. For calculation of structures the following groups of models are used: the balance models [2,3], regression models [4], one-dimensional kinematic models of the pollutant transfer in structures [5,6,7]. These models are economical and simple for practical application. However, a serious drawback of these groups of models is that *they do not take into account the geometric shape of the settler* or its other design features (e. g., partitions inside the structure). The use of one-dimensional kinematic models for the calculation of settlers with a complex geometric shape is impossible. Taking into account the settler geometry can only be achieved by using 2D or 3D models. Application of multidimensional models for settler calculations requires a necessary solution of the hydrodynamic problem of determining the velocity field for the flow inside the settler. Abroad, to solve the hydrodynamic problem the model of a viscous fluid is usually applied (Navier – Stokes equation). Implementation of this CFD model requires a very fine grid, which is the cause for spending a lot of time on getting the result. A strong substantiation for the turbulence model application is also required for calculation of this class of flows. It should be noted that calculation of the settler on the basis of a specialized code that realizes CFD model costs more than 20 thousand dollars abroad. [8]. In Ukraine, multi-dimensional CFD models for vertical settler calculations are practically not being developed. Therefore, development of effective methods for the calculation of vertical settlers, based on the application of CFD models and allowing prompt, low-cost calculation of the structures having complex geometry is a problem of current importance.

The aim of the research is elaboration of 3D CFD model of mass transfer in the vertical settler, which allows taking into account geometry of the settler during modeling. It should be noted that in [9, 10] 2D CFD model of the vertical settler calculation is presented.

Mathematical model of mass transfer process in a vertical settler

The process of pollutant transport inside a vertical settler is calculated on the basis of three-dimensional contaminant transfer equation [11]:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}+\frac{\partial (w-w_s)C}{\partial z}+\sigma C=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu_z\frac{\partial C}{\partial z}\right), \qquad (1)$$

where C is the pollutant concentration in the water; u, v, w – the flow velocity vector components;

μ_x, μ_y, μ_z – diffusion coefficients; t - time; w_s – the pollutant sedimentation rate; σ - factor taking into account the processes of agglomeration, etc., in the settler.

Boundary conditions for the transfer equation

The walls of the settler and various impenetrable objects within it (the tube, partitions, etc.) are the boundary lines of the current. In the numerical model built on these boundaries boundary condition of the following form is realized:

$$\frac{\partial C}{\partial n} = 0,$$

where n is a unit vector of the external normal to the solid surface.

The numerical model realizes boundary condition of the pollutant “absorption” on the solid horizontal surfaces of the settler. At the input boundary (at the boundary of the waste water flow input into the settler) the following condition is imposed:

$$C\Big|_{boundary} = C_E,$$

where C_E is a known value of the pollutant concentration.

The numerical model imposes a “cyclic” (soft) boundary condition at the output boundary of the computational region:

$$C(i+1, j, k) = C(i, j, k),$$

where i, j, k are the differential cell numbers.

At the initial moment it is assumed that $C = 0$ in the computational region. The problem of the pollutant distribution in the settler is solved for establishing the solution.

Model of hydrodynamics

To solve the equation of the pollutant transfer in the settler (1) is possible if the field of the flow rate in the vertical settler is known. Therefore, for the calculation of pollutant transport in the settler it is necessary to solve the hydrodynamic problem and to determine this field. To solve this hydrodynamic problem, a 3D model of potential flow is used. In this case, the model equation is given by [12]:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2} = 0, \qquad (2)$$

where P is velocity potential.

For equation (2) the following boundary conditions are set [12]:

- on the solid walls of the settler, on the partitions inside it: $\frac{\partial P}{\partial n} = 0$, where n is a unit vector of the external normal to the solid boundary;

- at the input boundary (region of the waste water inflow to the settler): $\frac{\partial P}{\partial n} = V_n$, where V_n - the known value of the inflow velocity;

- at the output boundary of the computational region (region of the clarified water outflow from the settler) $P = P*(x = const, y) + const$. (Dirichlet condition).

After calculation of the velocity potential field, calculation of the components of the waste water flow rate is performed on the basis of the dependencies [5]:

$$u = \frac{\partial P}{\partial x}, \qquad v = \frac{\partial P}{\partial y}, \qquad w = \frac{\partial P}{\partial z}.$$

Numerical method for solving the pollutant transfer equation

For numerical integration of the equation of the pollutant transfer in the settler a triangular differential splitting scheme is interchangeably used [13,14]. The numerical calculation is implemented on a rectangular difference grid. The concentration of the pollutant is calculated in the centers of differential cells. Let us consider the construction of the differential scheme for the transfer equation.

Let us replace the time derivative by the divided difference "backwards" (introduced according to "k").

$$\frac{\partial C}{\partial t} \approx \frac{C_{i,j,k}^{n+1} - C_{i,j,k}^{n}}{\Delta t}.$$

Convective derivatives are represented in the form of

$$\frac{\partial uC}{\partial x} = \frac{\partial u^{+}C}{\partial x} + \frac{\partial u^{-}C}{\partial x},$$

$$\frac{\partial vC}{\partial y} = \frac{\partial v^{+}C}{\partial y} + \frac{\partial v^{-}C}{\partial y},$$

$$\frac{\partial wC}{\partial z} = \frac{\partial w^{+}C}{\partial z} + \frac{\partial w^{-}C}{\partial z},$$

where $u^{+} = \dfrac{u+|u|}{2}$; $u^{-} = \dfrac{u-|u|}{2}$; $v^{+} = \dfrac{v+|v|}{2}$; $v^{-} = \dfrac{v-|v|}{2}$; $w^{+} = \dfrac{w+|w|}{2}$; $w^{-} = \dfrac{w-|w|}{2}$.

Let us perform approximation of the convective derivatives by the divided differences "upstream":

$$\left.\begin{aligned}
\frac{\partial u^{+}C}{\partial x} &\approx \frac{u_{i+1,j,k}^{+} C_{i,j,k}^{n+1} - u_{i,j,k}^{+} C_{i-1,j,k}^{n+1}}{\Delta x} = L_x^{+} C^{n+1}, \\
\frac{\partial u^{-}C}{\partial x} &\approx \frac{u_{i+1,j,k}^{-} C_{i+1,j,k}^{n+1} - u_{i,j,k}^{-} C_{i,j,k}^{n+1}}{\Delta x} = L_x^{-} C^{n+1}, \\
\frac{\partial v^{+}C}{\partial y} &\approx \frac{v_{i,j+1,k}^{+} C_{i,j,k} - v_{i,j,k}^{+} C_{i,j-1,k}}{\Delta y} = L_y^{+} C^{n+1}, \\
\frac{\partial v^{-}C}{\partial y} &\approx \frac{v_{i,j+1,k}^{-} C_{i,j+1,k} - v_{i,j,k}^{-} C_{i,j,k}}{\Delta y} = L_y^{-} C^{n+1}, \\
\frac{\partial w^{+}C}{\partial z} &\approx \frac{w_{i,j,k+1}^{+} C_{i,j,k} - w_{i,j,k}^{+} C_{i,j,k-1}}{\Delta z} = L_z^{+} C^{n+1}, \\
\frac{\partial w^{-}C}{\partial z} &\approx \frac{w_{i,j,k+1}^{-} C_{i,j,k+1} - w_{i,j,k}^{-} C_{i,j,k}}{\Delta z} = L_z^{-} C^{n+1}.
\end{aligned}\right\}$$

The second derivatives are approximated as follows:

$$\frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) \approx \tilde{\mu}_x \frac{C_{i+1,j,k}^{n+1} - C_{i,j,k}^{n+1}}{\Delta x^2} - \tilde{\mu}_x \frac{C_{i,j,k}^{n+1} - C_{i,j-1,k}^{n+1}}{\Delta x^2} = M_{xx}^{-} C^{n+1} + M_{xx}^{+} C^{n+1},$$

$$\frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) \approx \tilde{\mu}_y \frac{C_{i,j+1}^{n+1} - C_{i,j}^{n+1}}{\Delta y^2} - \tilde{\mu}_y \frac{C_{i,j}^{n+1} - C_{i,j-1}^{n+1}}{\Delta y^2} = M_{yy}^{-} C^{n+1} + M_{yy}^{+} C^{n+1}.$$

In the expressions used above L_x^+, L_x^-, M_{xx}^+, M_{xx}^-, etc. are designations of difference operators. Taking into account these designations, difference analog of the pollutant transfer equation will be given by:

$$\frac{C_{i,j,k}^{n+1}-C_{i,j,k}^{n}}{\Delta t}+L_x^+C^{n+1}+L_x^-C^{n+1}+L_y^+C^{n+1}+L_y^-C^{n+1}+L_z^+C^{n+1}+L_z^-C^{n+1}+\sigma C_{i,j,k}^{n+1}=$$
$$=\left(M_{xx}^+C^{n+1}+M_{xx}^-C^{n+1}+M_{yy}^+C^{n+1}+M_{yy}^-C^{n+1}+M_{zz}^+C^{n+1}+M_{zz}^-C^{n+1}\right).$$

For integration in time interval ∂t, we break up the solution of this difference equation in the following way:

at the first step $k=\frac{1}{4}$:

$$\frac{C_{i,j}^{n+k}-C_{i,j}^{n}}{\Delta t}+\frac{1}{2}\left(L_x^+C^k+L_y^+C^k+L_z^+C^k\right)+\frac{\sigma}{4}C_{i,j,k}^{k}=$$
$$=\frac{1}{4}\left(M_{xx}^+C^k+M_{xx}^-C^n+M_{yy}^+C^k+M_{yy}^-C^n+M_{zz}^+C^k+M_{zz}^-C^n\right), \tag{3}$$

at the second step $k=n+\frac{1}{2}$; $c=n+\frac{1}{4}$:

$$\frac{C_{i,j,k}^{k}-C_{i,j,k}^{c}}{\Delta t}+\frac{1}{2}\left(L_x^-C^k+L_y^-C^k+L_z^-C^k\right)+\frac{\sigma}{4}C_{i,j}^{k}=$$
$$=\frac{1}{4}\left(M_{xx}^-C^k+M_{xx}^+C^c+M_{yy}^-C^k+M_{yy}^+C^c+M_{zz}^-C^k+M_{zz}^+C^c\right), \tag{4}$$

at the third step $k=n+\frac{3}{4}$; $c=n+\frac{1}{2}$ formula (4) is used;

at the fourth step $k=n+1$; $c=n+\frac{3}{4}$ formula (3) is used.

In the above designations it is assumed that $w=w-w_s$.

The unknown value of the pollutant concentration is determined by the explicit point-to-point computation formula at each step of the break-up.

Numerical integration of the equation for the velocity potential

For numerical integration of equation (2) the method of Liebmann is used. In this case the approximation equation is given by:

$$\frac{P_{i+1,j,k}-2P_{i,j,k}+P_{i-1,j,k}}{\Delta x^2}+\frac{P_{i,j+1,k}-2P_{i,j,k}+P_{i,j-1,k}}{\Delta y^2}+\frac{P_{i,j,k+1}-2P_{i,j,k}+P_{i,j,k-1}}{\Delta z^2}=0.$$

On the basis of this dependence we obtain the formula for the velocity potential in the centre of the difference cell:

$$P_{i,j,k}=\left[\frac{P_{i+1,j,k}-P_{i-1,j,k}}{\Delta x^2}+\frac{P_{i,j+1,k}-P_{i,j-1,k}}{\Delta y^2}+\frac{P_{i,j,k+1}-P_{i,j,k-1}}{\Delta z^2}\right]\Big/A,$$

where $A=\left(\frac{2}{\Delta x^2}+\frac{2}{\Delta y^2}+\frac{2}{\Delta z^2}\right)$.

The calculated field of the velocity potential is used to determine the velocity vector components at the faces of the control volumes (difference cells) by the formulas:

$$u_{i,j,k} = \frac{P_{i,j,k} - P_{i-1,j,k}}{\Delta x},$$

$$v_{i,j,k} = \frac{P_{i,j,k} - P_{i,j-1,k}}{\Delta y},$$

$$w_{i,j,k} = \frac{P_{i,j,k} - P_{i,j,k-1}}{\Delta z}.$$

Calculation of the flow rate vector components on the faces of the difference cells makes it possible to build a conservative difference scheme for the equation of the pollutant transfer inside the settler. Numerical calculation of the velocity field and the pollutant transfer process in the vertical settlers is performed in the area of the complex geometric shape. Formation of the settler geometry on the rectangular difference grid is realized using the method of labeling [13]. This approach allows the user to form any geometry of the settler with no restrictions imposed on it.

Practical implementation of the model

On the basis of the constructed CFD model a specialized code «Settler-3D» has been developed. For programming *FORTRAN* was used.

The constructed numerical model was used for simulating the mass transfer process in a vertical settler with a partition (Fig.1) [2]. *The aim of the computational experiment* is estimation of the efficiency of water purification in the settler of the type under consideration for different pollutant settling rates w_s and for different location of the partition inside the settler.

Computational experiment was conducted for the following parameters: the settler length – 6 m; the width – 5 m; the depth - 3,34 m; flow rate at the settler input - 12 m/h; diffusion coefficient in all coordinate directions – 0,7 m^2/h; w_s =1,6 m/h и w_s =0,5 m /h; k =0. Pollutant concentration in the inflow to the settler is 100 units. (in a dimensionless form). The partition length is 1, 66 m.

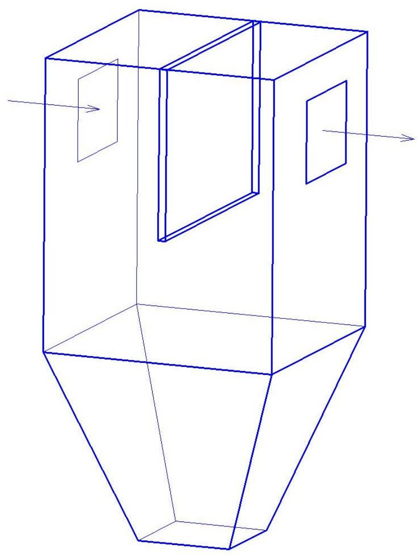

Fig. 1. Scheme of the vertical settler with a partition

Let us consider the results of the computational experiment. Fig. 1 presents distribution of the value of the pollutant concentration in the settler (side view) for cross-section y =2,25 m, w_s =1,2 m/h. In this variant of the problem the partition is located in the middle of the settler. This drawing shows where the input and the output of the flow take place. For the comparison, fig. 3 presents the pollutant concentration distribution for the same cross-section of the settler but for the pollutant settlement rate w_s =0,5 m/h. It can be seen clearly that for the parameter value w_s =1,2 m/h the pollutant concentration distribution along the settler height is significantly uneven: the most of the pollutant mass is concentrated in the downstream part of the settler while in the upstream flow the pollutant concentration is considerably less (contamination zone in this part of the settler seems to be “dispersed”).

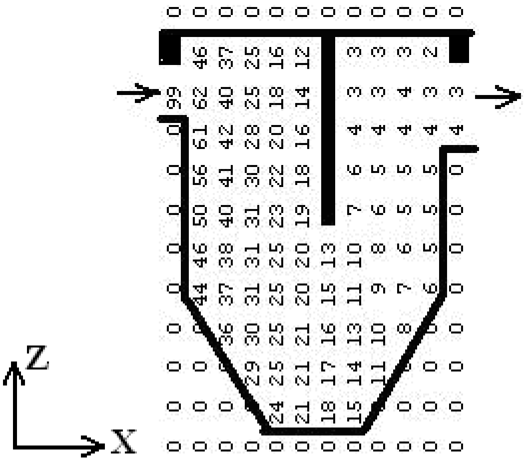

Fig. 2. The pollutant concentration distribution in the vertical settler with a partition (side view, cross-section y =2,25m, w_s =1,2m / h, $C_{\max}$ =100)

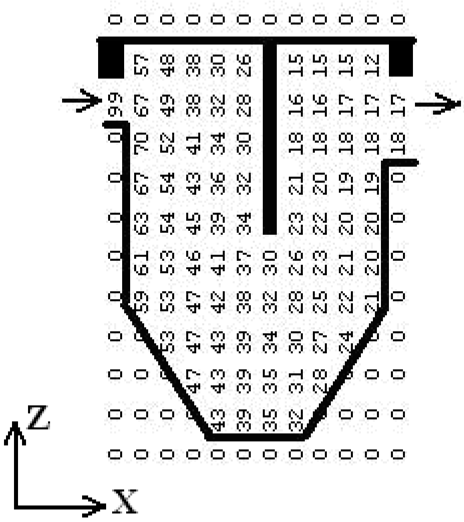

Fig. 3. The pollutant concentration distribution in the vertical settler with a partition (side view, cross-section y =2,25 m, w_s = 0,5 m / h, $C_{\max}$ =100)

For the value w_s =0,5 m/h the pollutant concentration value for this cross-section is different, more even, which is a clear evidence of the less effective water purification process. The subsequent figures show the pollutant concentration distribution for different cross-sections of the settler for the value of w_s =1,2 m/h. These data enable purification effectiveness evaluation for different parts of the settler. Fig. 6 presents the pollutant concentration distribution in the settler for the variant when the partition is shifted closer to the outlet of the structure.

It should be stressed that in the presented drawings the concentration value is represented in a dimensionless form: each number is the value of concentration as a percentage of the maximal concentration for this cross-section. Therefore, below each of the figures information is given about the maximal concentration value for this cross-section. Such representation of the computational experiment results enables prompt analysis of the information on the estimated value of concentration in any part of the settler. It should be noted that the calculation results are printed in the format of “integer “ numbers, i. e. the fractional part of the number is not given to the printer. This means that if, for example, at some point the calculated concentration value is "1.85%" of the concentration at the inlet to the settler, the printer will print "1". Similarly, if the concentration value is less than 1 %, then “0” will be printed. This approach to the form of printing the results is effective for series calculations when various variants are considered in order to choose the most optimal structure design. For a detailed analysis of the calculation data the developed code gives the concentration value in the format of “real” numbers, i.e. with preservation of the fractional part value.

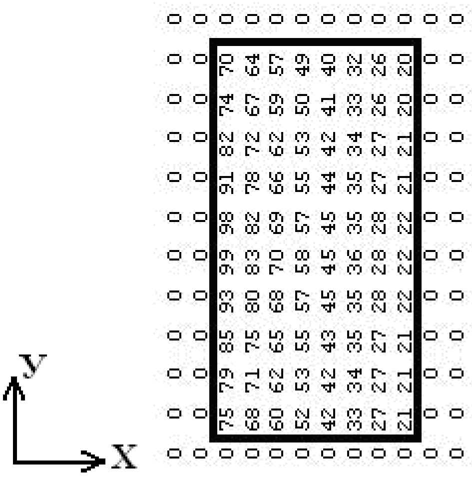

Fig. 4. The pollutant concentration distribution in a vertical settler with a partition (top view, cross-section z =0,82 m, w_s =1,2 m / h, $C_{\max}$ =0,3)

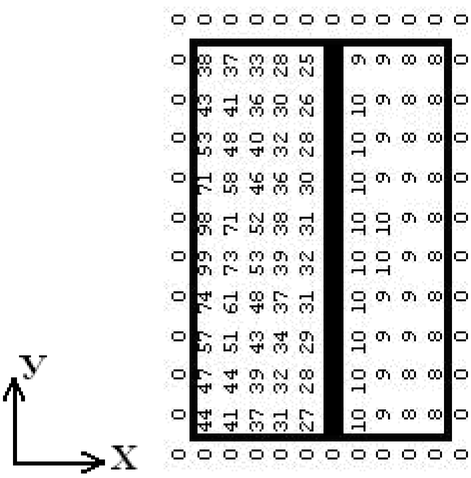

Fig. 5. The contaminant concentration distribution in a vertical settler with a partition (top view, cross-section z =2,14 m, w_s =1,2 m / h, $C_{\max}$ =0,52)

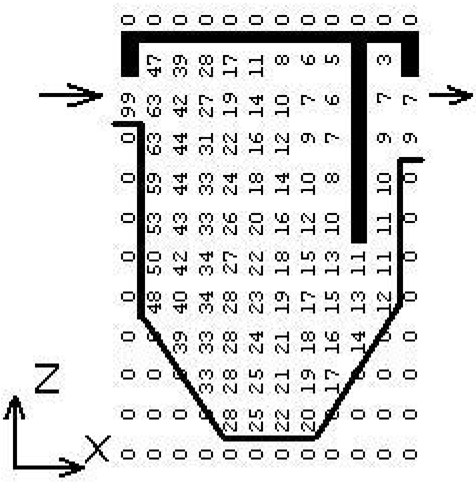

Fig .6. The pollutant concentration distribution in a vertical settler with a partition shifted to the outlet (side view, cross-section y =2,25 m, w_s =1,2m / h, $C_{\max}$ =100).

On the basis of the computational experiment the efficiency of the settler operation is determined. Accordingly, the value of the pollutant concentration at the settler outlet (the purification efficiency) for the value of w_s =1,2 m / h, is $C_{\hat{a}}$=2 % of the value of the pollutant concentration at the settler inlet while for the value w_s =0,5 m /h, the pollutant concentration at the settler outlet is $C_{\hat{a}}$=13 – 15 %. Thus, reduction of the pollutant settlement rate by about 2,4 times resulted in the significant deterioration (about 7 times) of the degree of water purification in the settler. For the settler with the partition shifted to the outlet (w_s =1,2 m / h), the pollutant concentration at the settler outlet is $C_{\hat{a}}$=3 %.

In conclusion it should be noted that calculation of one variant of the problem has taken about 2 minutes of computer time. Such minimal time spent on the computational experiment is an important factor in performing serial calculations in practice.

Conclusions

The paper presents an effective 3D numerical model for studying the mass transfer process in vertical settlers with complex geometry. The created specialized code can be used as a tool for solving a complex of applied problems evolving during design and reconstruction of vertical settlers. The constructed numerical model is distinguished by operative calculation of structures in 3D statement. Further work should be directed towards the development of the model of mass transfer in settlers based on the model of separated vortex flows of ideal fluid.

REFERENCES

1. Vanrolleghem P. A. New measurement techniques for secondary settlers: a review / P. A. Vanrolleghem, B. D. Clercq, J. D. Clercq, M. Devisscher, D. J. Kinnear, I. Nopens // Water Science & Technology, 2006. – Vol 53, No 4 – 5. – P. 419 – 429.

2. Таварткиладзе И. М. Математическая модель расчета вертикальных отстойников с перегородкой / И. М. Таварткиладзе, А. М. Кравчук, О. М. Нечипор // Водоснабжение и санитарная техника. – Вып. № 1. – 2006. – Ч. 2. – С. 39 – 42.

3. Stamou A. I. Validation and application of a simple model for circular secondary settling tanks / A. I. Stamou, D. L. Giokas, Y. Kim, P. A. Paraskevas // Global NEST Journal. – Greece, 2008. – Vol 10, No 1. – P. 62 – 72.

4. Токарь И. Я. К расчету вертикальных отстойников водоочистных сооружений / И. Я. Токарь, Г. И. Сухоруков, Д. Г. Сухоруков // Науковий вісник будівництва. – № 59. – 2010. – С. 293 – 296.

5. Олейник А. Я. Теоретический анализ процессов осаждения в системах биологической очистки сточных вод / А. Я. Олейник, Ю. И. Калугин, Н. Г. Степовая, С. М. Зябликов // Прикладная гидромеханика. – Том 6 (78). – № 4. – 2004. – С. 62 – 67.

6. Степова Н. Г. До розрахунку вертикального відстійника з урахуванням форми його нижньої частини / Н. Г. Степова, Ю. І. Калугін, О. Я. Олійник // Проблеми водопостачання, водовідведення та гідравлики. – Вип. № 14. – 2010. – С. 145 – 151.

7. Stamou A. I. A 1-D model for secondary circular clarifiers / A. I. Stamou // Proc. of the Intern. Conference for the Restoration and Protection of the Environment V, Mykonos, Greece, 2004. – P. 8

8. Shaw A. Optimizing Energy Dissipating Inlet (Edi) Design In Clarifiers Using An Innovative CFD Tool / A. Shaw, S. McGuffie, C. Wallis-Lage, J. Barnard // WEFTEC, 2005. – P. 8719 – 8736.

9. Беляев Н. Н. Математическое моделирование работы канализационного отстойника / Н. Н. Беляев, Е. К. Нагорная // Проблемы и перспективы развития железнодорожного транспорта: 72 міжн. наук.-практ. конф., 19 –20 квітня 2012 р.: тези доп. – Дніпропетровськ, 2012. – С. 209 – 210.

10. Беляев Н. Н. Численная модель работы вертикального отстойника / Н. Н. Беляев, Е. К. Нагорная // Современные информационные технологии на транспорте, в промышленности и образовании: межд. научн.-практ. конф., 5 – 6 квітня 2012 р.: тезисы докл. – Днепропетровск, 2012. – С. 56.

11. Марчук Г. И. Математическое моделирование в проблеме окружающей среды / Г. И. Марчук. – М.: Наука, 1982. – 320 с.

12. Лойцянский Л. Г. Механика жидкости и газа / Л. Г. Лойцянский. – М.: Наука, 1978. – 735 с.

13. Згуровский М. З. Численное моделирование распространения загрязнения в окружающей среде / М. З. Згуровский, В. В. Скопецкий, В. К. Хрущ, Н. Н. Беляев. – К.: Наук. думка, 1997. – 368 с.

14. Беляев Н. Н. Компьютерное моделирование динамики движения и загрязнения подземных вод. / Н. Н. Беляев, Е. Д. Коренюк, В. К. Хрущ. – Днепропетровск: Наука и образование, 2001. – 156 с.

15. Самарский А. А. Теория разностных схем / А. А. Самарский. – М.: Наука, 1983. – 616 с.

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