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SIMULATION OF WATER FLOW IN A CAVITATION REACTOR

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Abstract
Introduction: Searching for methods to improve the efficiency of water treatment with reagents is quite important in both water conditioning and industrial wastewater purification. Among the technologies providing high efficiency and reducing resource consumption in combination with reagent methods, hydrodynamic cavitation water treatment is of particular interest. The analysis of scientific and technical data made it possible to determine the main indicators of hydrodynamic cavitation water treatment that can affect the efficiency of reagent purification. Extreme parameters occurring during intense cavitation are associated with the formation of high temperatures up to 2000°C and high pulse pressures of 100–1500 MPa in local areas of hydrodynamic systems. In such conditions, the initiation and intensification of the physical and chemical processes of water treatment are observed. **Purpose of the study:** Improving the efficiency of existing traditional water purification technologies, allowing to improve its quality at the lowest cost. **Methods:** To study the parameters affecting water treatment efficiency and occurring with the cavitation flow of water, simulation in Ansys CFX was performed with the use of the finite volume method. The calculation was carried out with account for the turbulent nature of the flow based on the k-ε turbulence model. The cavitation process was calculated with the use of the Rayleigh-Plesset cavitation model. **Results:** Steam formation in the cavitation reactor promotes sufficiently complete absorption of the gaseous disinfectant by water. An increase in temperature is also considered as one of the factors increasing the efficiency of water treatment with reagents. During cavitation, water temperature increases in local micro-volumes. Thus, to intensify the process, there is no need to heat the entire volume of liquid, and, as a result, the total energy consumption for water treatment is reduced.

Keywords: cavitation reactor, cavitation parameters, water treatment processes, simulation.

Introduction

Since clean water is becoming one of the most valuable and expensive natural resources, great attention has been recently paid to the issues of drinking water treatment and industrial wastewater treatment. The current trends are moving in the direction of tightening regulatory requirements for the quality of water used for various purposes. That is why specialists focus on enhancing the efficiency of the existing traditional water purification technologies, which will make it possible to improve water quality in the least-cost manner.

To achieve those goals, in terms of environmental, process, and operational advantages, the use of physical methods seems the most appropriate. To increase the efficiency of processes and, as a consequence, reduce operating costs, it is required to develop and utilize efficient devices characterized by relatively low energy and material consumption and ensuring intensive impact on the treated medium. The development of devices providing energy impact on the treated media due to the pulsed flow conditions is one of the promising technical directions in purification intensification. Such devices include hydrodynamic cavitation reactors where the intensification of processes is provided by special flow conditions with mechanical and acoustic effects (Carpenter et al., 2017; Holkar et al., 2019; Pandit et al., 2021; Patil et al., 2021).

Extreme parameters occurring during intense cavitation are associated with the formation of high temperatures up to 2000°C and high pulse pressures of 100–1500 MPa in local areas of hydrodynamic systems (Belyaev and Flegentov, 2014; Chandra et al., 2019). In such conditions, the initiation and intensification of the physical and chemical processes of water treatment are observed. The authors conducted numerous experimental studies confirming the possibility of intensifying water treatment with reagents by applying hydraulic cavitation in a flow reactor. Those studies were carried out both during water conditioning and wastewater treatment (water disinfection by ozonation and chlorination (Belyaev and Flegentov, 2014); silica removal from water with magnesium oxide (Gimranov et al., 2014b), swimming pool water disinfection (Lysov et al., 2016), removal of phenol and petroleum products (Kuts, 2003), ammonium compounds from water (Gimranov et al., 2013)).

The technology for removal of organic compounds from water with simultaneous water disinfection can be improved by intensifying the mixing of disinfectant (ozone, chlorine) with treated water through the use of hydrodynamic cavitation (Belyaev and Flegentov, 2014; Belyaev et al., 2012; Fleguentov et al., 1997; Gogate et al., 2014). This technology can improve the quality of water treatment at water treatment facilities and in industrial wastewater treatment systems of chemical and machine-building enterprises, thermal power and other plants. Intensification of mixing two-phase flows by hydrodynamic cavitation can also be used to reduce disinfectant consumption when introducing it into the treated water at water purification plants (Belyaev et al., 2012).

The use of underground water sources for the needs of heat and power facilities as well as chemical and pharmaceutical, pulp and paper industry often requires silicon compounds to be removed from water in water conditioning (Huuha et al., 2010). Therefore, the search for ways to upgrade the existing technologies of silica removal from water and improve the efficiency of treatment with reagents in the applied technologies remains quite urgent. The authors also studied intensification of the process of silica removal from water of underground sources by its additional exposure to hydrodynamic cavitation in a flow reactor (Belyaev et al., 2019). It was established that the rate of silica removal from water using magnesium oxide with additional cavitation treatment increases by 17.1%.

The authors also studied the use of hydrodynamic cavitation to intensify swimming pool water purification (Gimranov et al., 2014a; Lysov et al., 2016). The possibility of obtaining aqueous suspensions of metals with oligodynamic effect by cavitation erosion was considered. The sizes of silver and copper particles formed during cavitation treatment in a hydrodynamic flow unit of original design were experimentally evaluated using a scanning microscope.

Subject and methods

We aimed to study the parameters occurring with the cavitation flow of water and affecting the efficiency of water conditioning and purification.

To do that, we considered the flow of water in a cavitation reactor, the parameters of which were proposed in the patent by Belyaev and Flegentov (2012) (Fig. 1). The flow of water in the unit was determined in Ansys CFX (Abdulin et al., 2011) with the use of the finite volume method (Zamankhan, 2015).

The calculation was carried out with account for the turbulent nature of the flow based on the k–ε turbulence model (Ranade, 2022). The cavitation process was calculated with the use of the Rayleigh-Plesset cavitation model (Hilgenfeldt et al., 1998). The differential equation serving as the basis of this model takes the following form:

$$R\frac{d^2R}{dt^2}+\frac{2}{3}\left(\frac{dR}{dt}\right)^2+\frac{2\sigma}{\rho R}=\frac{p_S-p}{\rho}, \qquad (1)$$

where R — the radius of a steam bubble formed during cavitation, m; t — time, s; σ — the coefficient of surface tension in a steam bubble at the liquid boundary, N/m; ρ — liquid density, kg/m^3; p_s — pressure of saturated vapors, Pa, (assumed to be equal to p_S = 3169 Pa); p — absolute pressure in the flow point, Pa.

In the model put in Ansys CFX, an approximate solution of Eq. (1) is used to determine the rate of steam bubble formation and collapse depending on the pressure difference in the right part. The average diameter of a steam bubble, taken as nominal, was assumed to be equal to 2·10^{-6} m (Rooze, 2012).

In each finite volume, it was assumed possible to find water and steam parameters at the same time, the proportions between which depend on the rate of vaporization, while water enters the reactor as a liquid.

Figs. 2 and 3 show the division into finite volumes. The number of division elements was m = 114061, and the number of nodes was n = 231263.

Along the solid walls, no-slip conditions and mesh refinement in the boundary layer were set. The number of boundary layers was 5, the element height in the boundary layer did not exceed 1 mm. A uniform velocity field was set at the inlet to the cavitation reactor, and zero relative pressure was set at the outlet from the cavitation reactor (Fig. 4). The calculation was performed at two water flow velocity modes at the inlet: at 15 and 23 m/s. The studies were carried out with a reactor previously used in other works (Belyaev and Flegentov, 2014; Belyaev et al., 2012; Fleguentov et al., 1997; Gimranov et al., 2013, 2014a, 2014b; Kuts, 2003), with parameters as per Fig. 1: H = h = D = 10 mm, b = 20 mm.

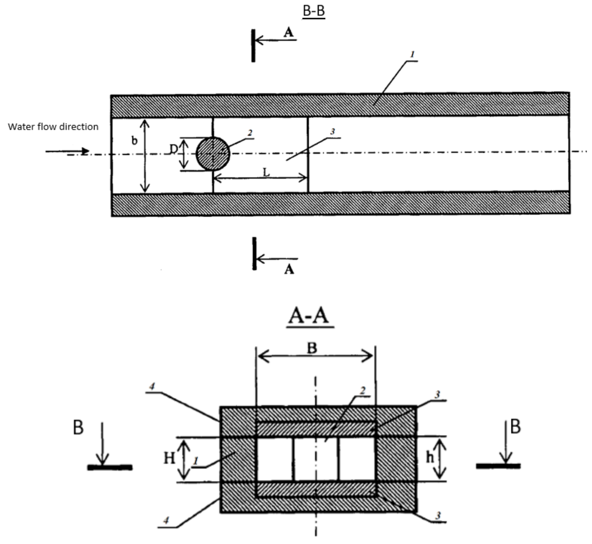

Fig. 1. Scheme of the cavitation reactor according to patent RU 2445272: 1 — walls of the reactor channel; 2 — a cylindrical cavitation exciter; 3 — metal substrates; 4 — a reactor vessel; H and D — height and diameter of the cavitation exciter, respectively; h and b — height and width of the cavitation channel, respectively; L — length of the metal substrate

Results and discussion

At the first stage of the calculations, we studied the flow of water without cavitation effect. Then the calculation results were set as initial conditions for the flow with account for cavitation.

As a result of the calculations, absolute pressure distribution fields were obtained, shown in Figs. 5 and 6.

It can be seen from the pressure distribution fields that pressure does not drop below the boiling point of water. The highest values *p* = 1.291 MPa (Fig. 5) and *p* = 0.5524 MPa (Fig. 6) are reached in front of the cylinder, and as the flow flows around, they drop to the boiling point *p* = 3169 Pa.

Figs. 7 and 8 show distribution of the volume fractions of steam in the flow.

Figs. 9 and 10 show distribution of the volume fractions of steam in the longitudinal section passing through the axis of the cylinder. The study of this parameter showed that boiling is more intense on the back side of the cylinder and at the channel walls behind it, which are parallel to the bases. It is expedient to install substrates with active materials for chemical reactions in these zones.

Figs. 11, 12, 13, and 14 show distribution of steam bubble and water velocities in the cavitation area.

Figs. 15–22 show distribution of the calculated values of steam and water temperature in the corresponding longitudinal sections of the reactor.

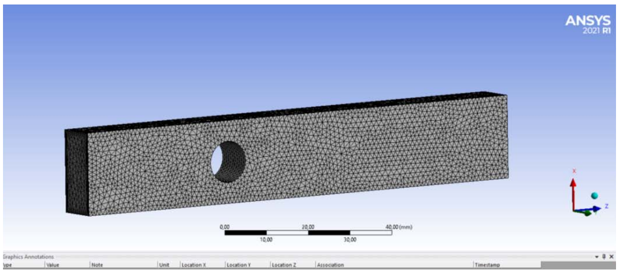

Fig. 2. Scheme of division into finite volumes

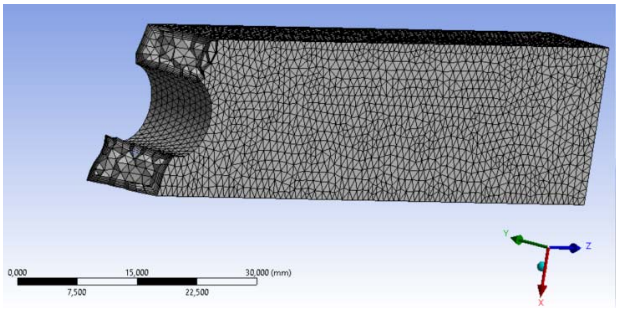

Fig. 3. Cross-section of the mesh model for visualization of the boundary layer

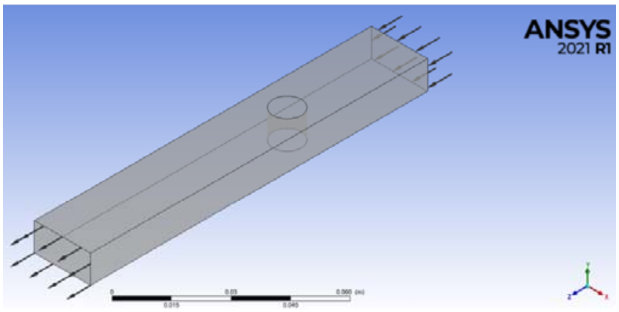

Fig. 4. Boundary conditions

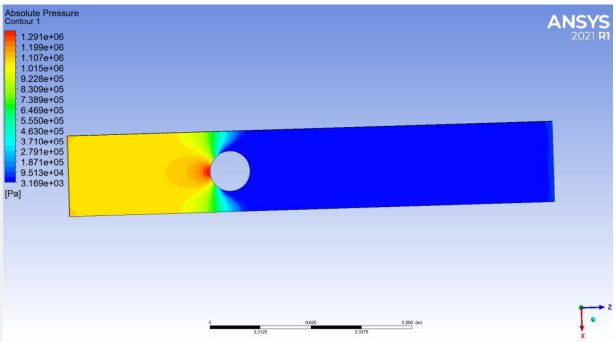

Fig. 5. Absolute pressure distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 23 m/s

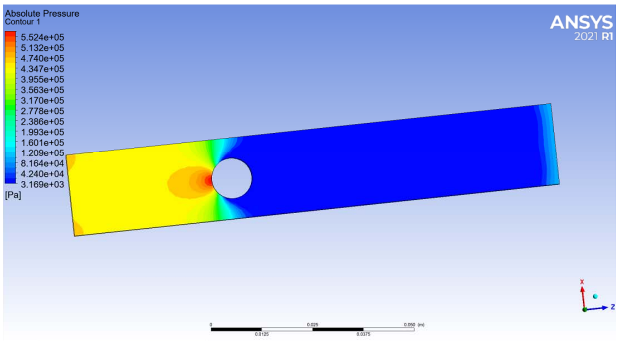

Fig. 6. Absolute pressure distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 15 m/s

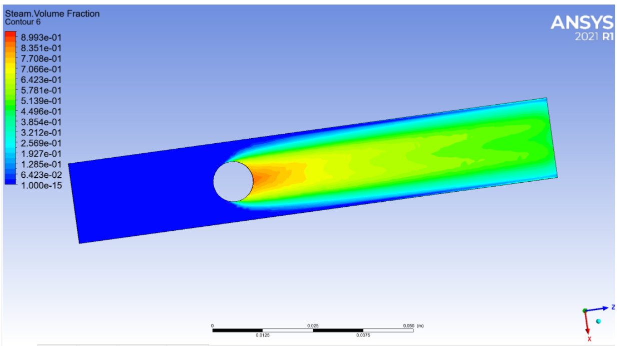

Fig. 7. Steam volume fraction distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 23 m/s

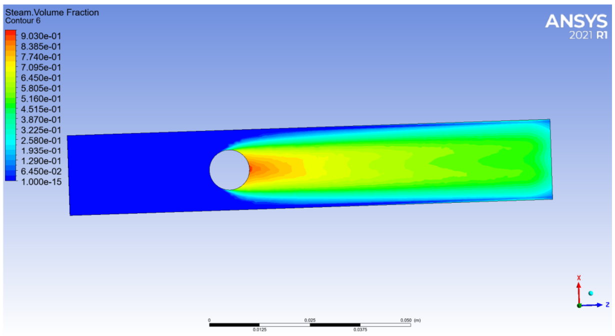

Fig. 8. Steam volume fraction distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 15 m/s

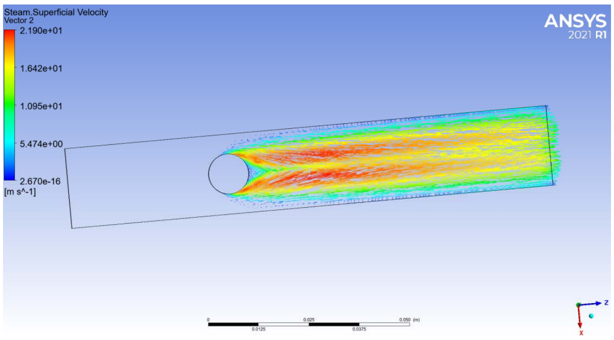

Fig. 12. Steam bubble velocity distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 15 m/s

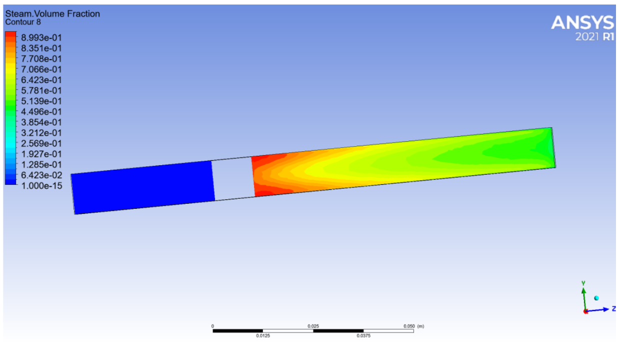

Fig. 9. Steam volume fraction distribution in the axial section of the cavitation reactor, passing through the axis of the cylinder at a water velocity at the inlet of 23 m/s

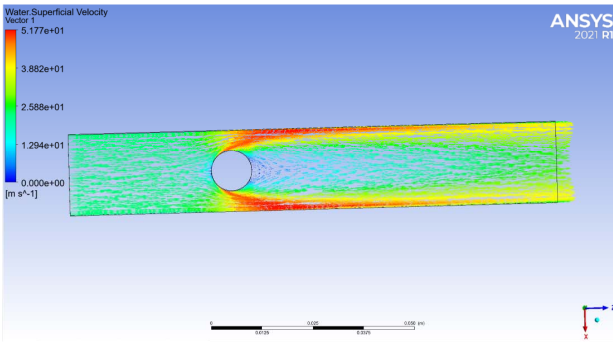

Fig. 13. Water velocity distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 23 m/s

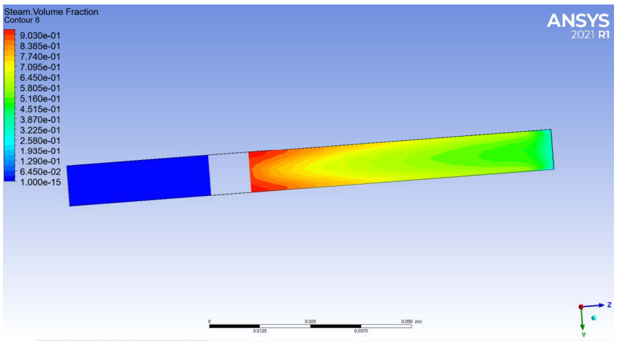

Fig. 10. Steam volume fraction distribution in the axial section of the cavitation reactor, passing through the axis of the cylinder at a water velocity at the inlet of 15 m/s

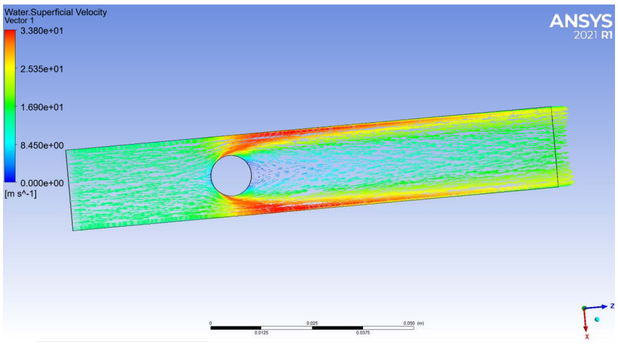

Fig. 14. Water velocity distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 15 m/s

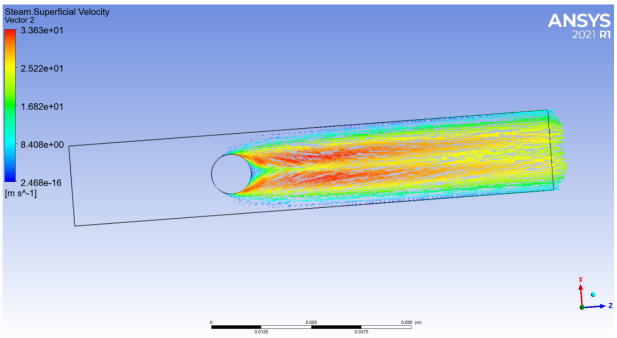

Fig. 11. Steam bubble velocity distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 23 m/s

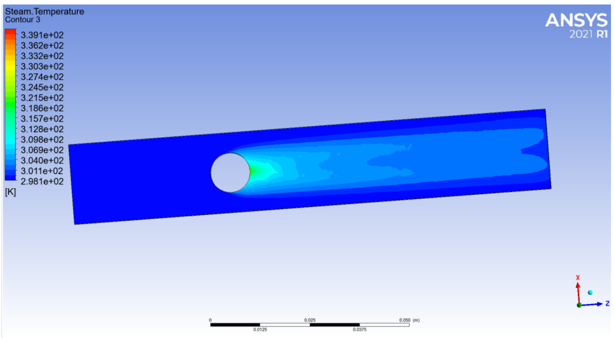

Fig. 15. Steam temperature distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 23 m/s

Let us take a look at a three-dimensional image of elements with a steam volume fraction of more than 0.7 (Figs. 23, 24)

With an increase in the input flow rate from 15 to 23 m/s, an increase in the length of the steam bubble plume is observed. Besides, there is a slight increase in the temperature of water in the flow when the absolute pressure required to create a velocity of 23 m/s is doubled.

The obtained results allow us to see the data obtained during field studies (conducted earlier with the use of the same cavitation reactor design) in the new light. For instance, in experiments to obtain aqueous suspension of silver (Gimranov et al., 2014a). Fig. 25 shows the surface of a silver substrate located at the base of the cavitation exciter.

On the left, we can see a plume of half of the base of the cylindrical exciter with a diameter of *D* = 8 mm; in the center, above and below, we can see clear outlines of an erosive plume from the cavitation torch, flowing around the exciter at a flow rate in the channel of 23 m/s. By comparing the sizes of this plume and distribution of the steam volume fraction in the axial section of the cavitation reactor, shown in Figs. 9 and 10, we can see a clear correspondence between the sizes of the red/orange zone (see Figs. 9–10) in the lower part of the channel and cavitation deformations observed at a distance up to 3*D*.

A more detailed study of erosive surfaces in the areas of initial deformation with the use of a JSM-6510 LV electronic scanning microscope (JEOL, Japan) with 500x magnification (Fig. 26) shows the presence of mechanical deformations caused by the separation of silver microparticles under the influence of water micro-jets due to the collapse of cavitation steam bubbles (Gimranov et al., 2014a). The thermal nature of the deformations in the image shall be ruled out with a high probability because of the absence of particular characteristic features.

The low effect of the temperature component on the cavitation deformations of the silver substrate is confirmed by images of temperature fields in the cavitation reactor, shown in Figs. 21 and 22. Here we can see the temperature dynamics in the cavitation zone at maximum deviation values of 43.6°C and maximum absolute value of 65.2°C, which is not sufficient for thermal deformations on the surface of the silver substrate. However, such dynamics causes changes in the cavitation conditions of the liquid flow in the reactor channel and contributes to the formation of cavitation cavities collapsing with an increase in pressure with the formation of micro-jets, thus facilitating the formation of erosive deformations.

In other studies on silica removal from water with magnesium oxide (Belyaev and Flegentov, 2014; Belyaev et al., 2019; Gimranov et al., 2014b) conducted with the use of the same cavitation reactor design (Belyaev and Flegentov, 2012), the

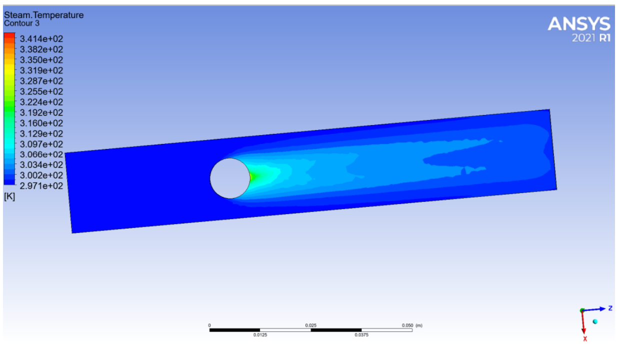

Fig. 16. Steam temperature distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 15 m/s

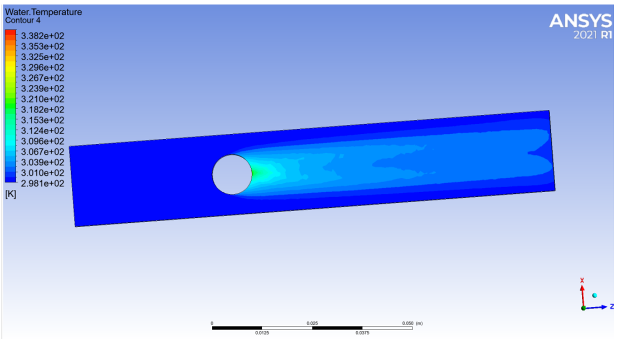

Fig. 17. Water temperature distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 23 m/s

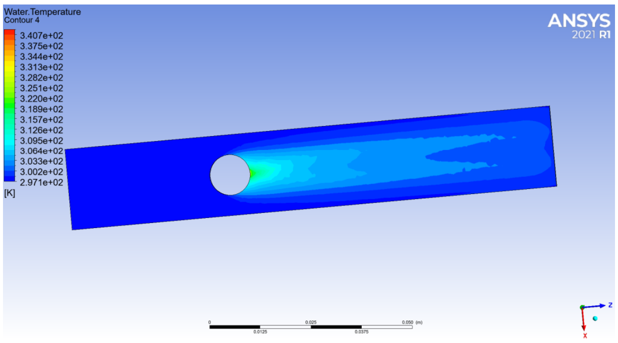

Fig. 18. Water temperature distribution in the axial section of the cavitation reactor, perpendicular to the axis of the cylinder at a water velocity at the inlet of 15 m/s

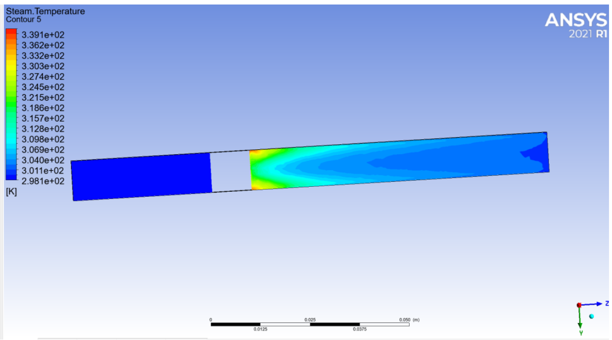

Fig. 19. Steam temperature distribution in the section of the cavitation reactor, passing through the axis of the cylinder at a water velocity at the inlet of 23 m/s

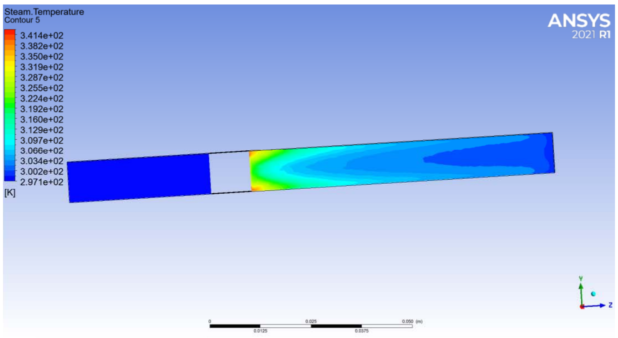

Fig. 20. Steam temperature distribution in the section of the cavitation reactor, passing through the axis of the cylinder at a water velocity at the inlet of 15 m/s

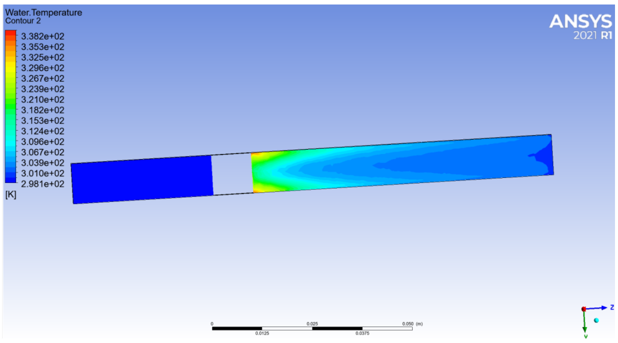

Fig. 21. Water temperature distribution in the section of the cavitation reactor, passing through the axis of the cylinder at a water velocity at the inlet of 23 m/s

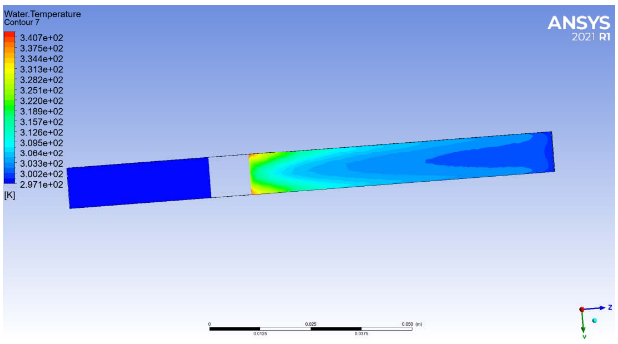

Fig. 22. Water temperature distribution in the section of the cavitation reactor, passing through the axis of the cylinder at a water velocity at the inlet of 15 m/s.

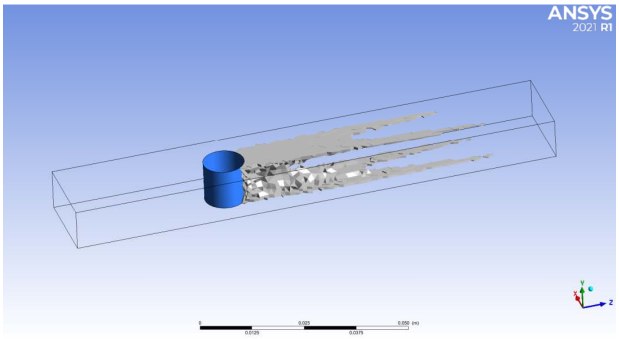

Fig. 23. Distribution of elements with a steam volume fraction of more than 0.7 in the cavitation reactor at a water velocity at the inlet of 23 m/s

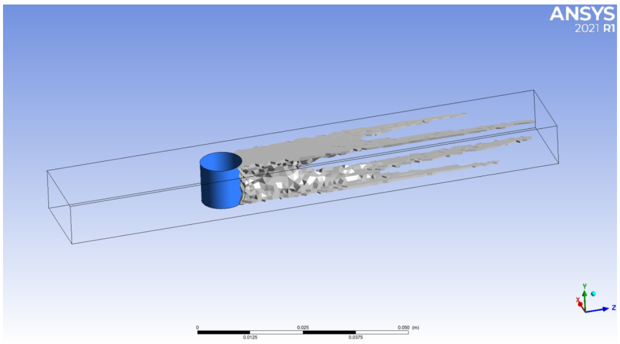

Fig. 24. Distribution of elements with a steam volume fraction of more than 0.7 in the cavitation reactor at a water velocity at the inlet of 15 m/s

Fig. 25. Silver substrate with traces of cavitation erosion

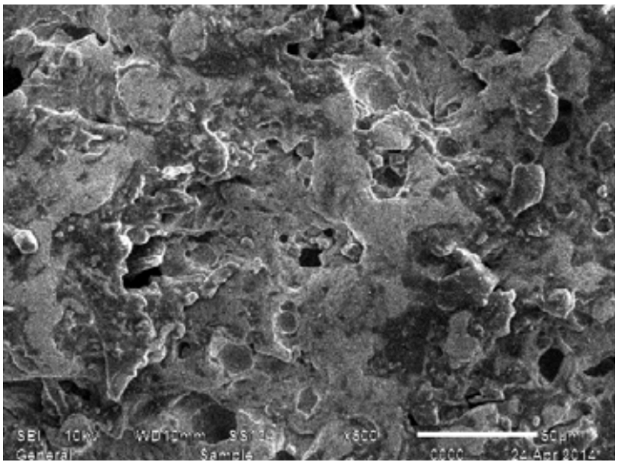

Fig. 26. Photo of the cavitation zone of the silver substrate at 500x magnification

temperature component had to play a key role in reaction intensification. In the course of the studies, the linear dependence between the changes in the rate of heating dynamics and the duration of treatment, expressed by the number of cycles, was determined. As a result, the dynamics of water heating per one cycle did not exceed 2.9°C at an initial temperature of 15°C (Belyaev and Flegentov, 2014). Its low values caused the need for multi-cycle treatment to obtain the required parameters necessary for efficient reactions during silica removal from water with magnesium oxide. This fact is also confirmed by the built model, which indicates the possibility of its use when applying cavitation in practice.

Conclusions

1. In the course of the study, we analyzed the parameters occurring with the cavitation flow of water and affecting the efficiency of water conditioning and purification. It was established that it is expedient to install substrates with active materials for chemical reactions on the back side of the cylindrical exciter and at the walls of the channel behind it, parallel to its bases, since intense boiling occurs in those very areas. The length of the zone is 7...9 cylinder diameters at water velocities at the inlet to the cavitation reactor of 15...23 m/s.

2. It is expedient to introduce liquid or gaseous reagents directly into the cavitation zone where pressure drop is the highest.

3. The resistance of the cavitation reactor increases significantly from 0.4 to 1.1 MPa with an increase in water velocity at the inlet from 15 m/s to 23 m/s, but the cavitation zone increases to a lesser extent, therefore, the rational value of velocity at the inlet is 15 ...18 m/s.

4. The increase in the flow temperature is most manifested in the section of the channel along the axis of the cylinder and along the walls parallel to its bases. The maximum value of 67°C is observed at the boundary of the back edge of the cavitation exciter and the side walls of the channel (at a water temperature at the inlet to the cavitator of 24°C)

5. In a cavitation reactor, the treated water flow passes through a zone with fast changes in velocities and pressures as well as fast formation and collapse of vapor/gas microspheres, which has a synergistic effect in water treatment technologies.

Thus, the use of highly intense cavitation in hydrodynamic flow units intensifies the physical and chemical processes of water purification and can be used in technologies of water treatment with reagents.

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МОДЕЛИРОВАНИЕ ТЕЧЕНИЯ ВОДЫ В КАВИТАЦИОННОМ РЕАКТОРЕ

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Аннотация
Введение: Поиск путей повышения эффективности реагентных методов обработки воды является актуальной задачей как в процессах водоподготовки, так и в процессах очистки производственных сточных вод. Среди технологий, способных в комплексе с реагентными методами обеспечить высокую производительность и снижение ресурсных затрат, особый интерес представляет гидродинамическая кавитационная обработка воды (ГДК). Анализ научно-технической информации позволил выделить основные показатели процесса гидродинамической кавитационной обработки воды, способные повлиять на эффективность процесса реагентной очистки. Экстремальные параметры, которые возникают при интенсивной кавитации, связаны образованием на локальном участке гидродинамической системы высоких температур до 2000 °С и импульсных давлений больших величин 100-1500 МПа. В таких условиях происходит инициация и интенсификация протекания физико-химических процессов обработки воды. **Цель исследования:** Повышение эффективности существующих традиционных технологий очистки воды, позволяющих улучшить ее качество с наименьшими затратами. **Методы:** Для исследования параметров, влияющих на эффективность процессов водоподготовки и возникающих при кавитационном течении воды было проведено моделирование в пакете Ansys CFX, в котором применен метод конечных объемов. Расчет проводился с учетом турбулентного характера течения по модели турбулентности k-ε. Процесс кавитации рассчитывался с использованием модели кавитации Релея-Плесета. **Результаты:** Процесс парообразования в кавитационном реакторе способствует достаточно полному поглощению газообразного дезинфектанта водой. Повышение температуры так же рассматривается как один из факторов повышения эффективности методов реагентной обработки воды. При кавитации повышение температуры воды происходит в локальных микрообъемах, поэтому для интенсификации процесса отсутствует необходимость осуществления нагрева всего объема жидкости и, как следствие, снижаются общие энергозатраты на процесс водоподготовки.

Ключевые слова: кавитационный реактор, параметры кавитации, процессы обработки воды, моделирование.