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REGULAR ARTICLE

Efficiency Analysis of Nanocoatings for Blade Surfaces in Vertical-Axis Underwater Turbines

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This study investigates the potential for improving the efficiency of vertical-axis underwater turbines by applying nanostructured coatings to blade surfaces. The proposed approach involves the formation of a simple periodic nanocoating composed of uniformly distributed cylindrical nanoparticles fixed on the surface. Using molecular dynamics simulations within the Gromacs framework and the coarse-grained Martini3 model, the interaction between a liquid flow and nanostructured surfaces was analyzed. The effects of the nanoparticles' diameter (10-50 nm), spacing (d – 5d), and height (0.5d – 2.5d) on the total hydrodynamic force acting on the surface at nanolevel were systematically studied. Two simulation strategies were considered: the application of an initial velocity impulse and the maintenance of a steady flow through a constant volumetric force. The results demonstrate that the relative force exerted by the flow depends strongly on the geometrical characteristics of the nanocoating. A distinct maximum was observed for particles with a diameter of approximately 20 nm, corresponding to a surface coverage of about 30-40 %. Increasing particle height enhances the transmitted force up to a certain limit, beyond which the effect saturates. Technological considerations indicate that coatings formed by deposition of near-spherical particles, where $h \approx d$, are the most feasible. Under such realistic conditions, the application of the nanocoating can increase the effective interaction force – and thus the flow energy conversion efficiency – by up to 20%. These findings suggest that nanostructured blade surfaces may represent a practical and cost-effective means to enhance the performance of underwater turbine systems.

Keywords: Surface nanostructure, Liquid-solid interaction, Water flow, Molecular dynamics, Coarse-grained modeling, Interaction efficiency.

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1. INTRODUCTION

In previous studies, the feasibility of employing underwater turbines with a vertical axis orientation for harvesting clean marine energy from water flows has been substantiated. When using a turbine-generator of any type, an important issue arises – improving its efficiency. Ideally, the turbine should extract the maxi-mum possible amount of energy from the incident flow of a continuous medium (whether gaseous or liquid). Naturally, there exists a certain upper limit to this extraction, determined by the fact that the flow cannot come to a complete stop after passing through the tur-bine – doing so would violate the continuity of mass flow – and therefore, not all the energy contained in the flow can be recovered.

As is well known, for horizontal-axis wind turbines (HAWTs), this theoretical limit was derived by Betz and equals $16/27 \approx 59.3\%$. However, for vertically oriented configurations (VAWTs), its calculation can yield different values – including values that may exceed Betz's limit for HAWTs, as will be shown through further analysis of available studies.

For example, in Newman's work [1], based on an original description of the airflow around a VAWT using an actuator disk model, the power coefficient (C_p) was found to be approximately 64%, indicating that vertically oriented turbines may possess even greater potential than their more traditional horizontal counterparts. It should be noted, however, that the actuator disk theory has certain limitations – as discussed, for instance, in [2] – and it is therefore reasonable to explore alternative approaches to evaluating the energy conversion efficiency of vertically oriented turbines.

In Helge Madsen's study [3], using the actuator cylinder model, the maximum C_p values were determined to be around 63%, which are consistent with results reported in his later publication [4].

In sources based on numerical modeling, even higher efficiency values have been reported. For instance, in [5], which employs the flux-line theory, a value of 66.4% is obtained, suggesting an even greater potential for VAWTs.

It should be noted, however, that despite the high

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theoretical efficiency coefficients reported for vertical-axis turbines, the actual performance indicators of existing technical implementations still lag significantly behind those of more traditional HAWTs. As summarized in the comprehensive review [6], the efficiency coefficients of vertical turbines may reach up to 31% (often remaining slightly below this value), whereas for industrial-scale HAWTs, the power coefficient typically exceeds 40%.

Similarly, in [7], which focuses on small and medium-sized wind installations, it is reported that the C_p value for vertical turbines remains below 0.4, while for advanced horizontal-axis turbines it can reach 0.5.

The results of wind tunnel experiments involving various turbine models presented in [8] also confirm this trend: HAWTs achieve C_p values of up to 50%, while VAWTs usually exhibit values in the range of 30–40% (it should be noted that this coefficient depends strongly on the specific design of the vertical turbine).

Comparable findings are also presented in numerous other studies, for example, [9-12].

These data indicate that vertically oriented tur-bines still possess significant untapped potential for improving their operational efficiency, which remains underutilized at the current stage of technological development. Therefore, it is reasonable to explore various technical solutions aimed at enhancing this efficiency coefficient.

One of the most straightforward approaches involves optimizing the aerodynamic shape of the tur-bine's flow-interacting elements (blades or vanes) to improve the conversion of flow energy into turbine rotation. However, other strategies for improving the overall process efficiency are also possible. In particular, one promising direction for further increasing the power coefficient C_p is the use of advanced materials (including metamaterials) or at least specialized surface coatings for turbine blades. Naturally, the influence of such materials or coatings must be substantiated through appropriate experimental studies or, at least at an initial stage, through numerical simulations.

2. METHODS

This study describes the possibility of enhancing the efficiency of flow energy conversion into turbine rotation by applying a geometrically simple nanocoating, consisting of nanoparticles with approximately cylindrical shapes fixed on the blade surface. The objective of this research is therefore to analyze the technical effective-ness of a nanocoating represented by uniformly distributed cylindrical nanoparticles on a flat turbine surface.

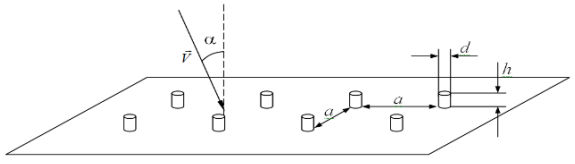


Fig. 1 – Schematic representation of the surface nanostructure and the parameters used for its description

To conduct this analysis, it is first necessary to de-fine the geometrical parameters of the proposed coating (see Fig. 1).

Three main surface coating parameters can be identified:

- the distance a between individual particle (with-out loss of generality, it is assumed that the grid is square);
- the height h of each particle above the flat surface;
- the diameter d of each particle.

Regarding the geometry of the particle arrangement on the surface, it should be noted that creating a uniform, regular grid of individual particles securely attached to the substrate is technologically challenging. The cost of producing such a regular array (for instance, by lithography and etching, or epitaxial growth) across the entire blade surface would be extremely high and could not be justified by any reasonable increase in tur-bine performance. A simpler and more practical approach, where the resulting particle distribution can be approximately modeled as periodic, is represented by deposition-based technologies (such as nanopowder spraying). This approach is relatively cost-effective; therefore, it will be assumed in the following analysis that the formation of the required nanostructure is technologically feasible, and the focus will be placed solely on assessing its performance (without considering the specific fabrication process).

In addition to surface parameters, the simulation must also account for flow characteristics, namely:

- the flow velocity V of the continuous medium impinging on the surface;
- the angle α between the flow direction and the normal to the surface.

When selecting suitable modeling tools, the following should be considered. Since the problem concerns the interaction of a liquid flow with a nanostructured surface, it requires specialized computational tools. Conventional Computational Fluid Dynamics (CFD) systems, such as ANSYS Fluent or OpenFOAM, cannot accurately capture nanoscale effects and are limited to surface features no smaller than approximately 1 μm. For significantly smaller structural elements, as in the present case, it is necessary to employ molecular modeling software, such as GROMACS or LAMMPS.

In the GROMACS molecular dynamics package [13], all computations are carried out within a closed simulation box (often shaped as a parallelepiped). Simulations can be performed with Periodic Boundary Conditions (PBC) either enabled or disabled. When PBC is active, any molecule leaving one side of the box reenters through the opposite side with the same velocity, there-by maintaining a constant number of molecules and ensuring model stability and continuity. When PBC is disabled, the number of molecules inside the simulation cell rapidly decreases, making the simulation physically inconsistent, since there is no mechanism to replenish lost molecules. Therefore, molecular modeling systems such as GROMACS require the use of periodically closed simulation domains, and the problem considered in this work thus necessitates the activation of PBC.

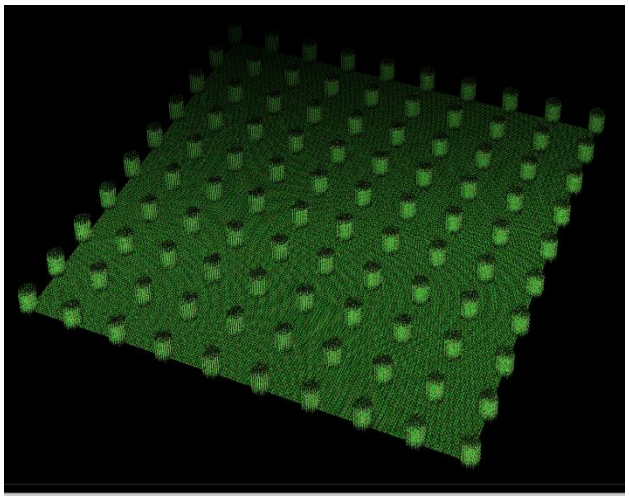
However, this introduces another difficulty related to maintaining a constant flow. Initially, all molecules can be assigned a macroscopic velocity component corresponding to the flow speed, consistent with the physical setup of the problem. Yet, molecules that have interacted with the surface lose part of their initial momentum; when they re-enter the simulation box through the periodic boundary, they no longer possess the original velocity distribution, thereby violating the problem's conditions (since molecules striking the surface now have a lower velocity than initially prescribed). To overcome this difficulty, two alternative strategies for conducting simulation experiments can be employed.

In the first simulation approach, it is necessary to accept the attenuation of the flow and to consider the action of a non-stationary flow on the nanostructured surface, characterized by having a defined velocity vector only at the initial moment of time. This corresponds to the interaction of the surface with an initial "impulse" that imparts kinetic energy to all water molecules, but whose effect is not sustained over time. The comparative efficiency of different surface coatings in terms of energy extraction from the flow can then be evaluated by the total force acting on all polymer atoms as a whole, averaged over an initial time interval of the simulation. This time interval should be short enough that the flow characteristics do not significantly deviate from their initial state. The relative efficiency of nanocoatings with different structures can be assessed by normalizing all absolute force values with respect to the minimum value obtained for one of the surface types (presumably, the uncoated surface).

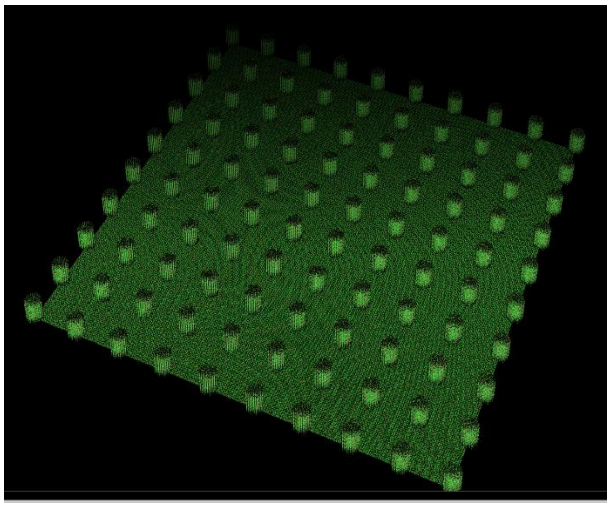
In the second approach, a constant volumetric force can be applied throughout the simulation domain to maintain a steady flow. However, establishing a pre-defined flow velocity using a specific volumetric force magnitude f can be challenging, since the direct functional dependence $V(f)$ is generally unknown. In practice, different values of f can be assigned, and the resulting flow velocity can then be determined experimentally during the simulation. In this context, the flow velocity may be understood as the average velocity of molecules entering the simulation cell through its inlet boundary.

Regarding the influence of the angle α on the magnitude of the force transmitted from the flow to the blade surface, this dependency is not a primary focus of the present study. During turbine operation, the blade surfaces continuously form varying angles with the flow direction, making it impossible to define or maintain a single fixed angle throughout the energy conversion process. The present work instead focuses on investigating whether the application of a nanocoating affects the interaction between the liquid flow and the surface. Consequently, the analysis will be limited to the influence of surface geometric parameters, while the flow characteristics will be fixed at representative mean values, for example, $\alpha = 20°$, $V = 1$ m/s (corresponding, for instance, to the typical velocity of water flow in the lower Danube river under strong current conditions).

Thus, to account for nanoscale effects in the interaction of water flow with a nanocoated surface, one must employ molecular modeling systems, which operate under periodic boundary conditions and a constant number of particles. These constraints necessitate finding ways to maintain a steady flow, achievable either over a short simulation time (approximating a quasi-stationary regime) or by applying a constant volumetric force to the solvent molecules, thereby generating a continuous flow. However, since the exact velocity of such a flow cannot be predicted a priori, it is preferable to study the coating's efficiency not by prescribing a specific flow velocity, but by setting the volumetric force magnitude and determining the corresponding surface force produced during simulation.



a



b

Fig. 2 – Visualization of the modeled system in the PyMOL program (solvent molecules – water – are not shown): initial structure (a), optimized structure after primary energy minimization (b)

When using nanoscale physical simulation software, another challenge arises: achieving an adequately large number of particles to ensure realistic modeling of the

system. This makes the computational task extremely demanding and typically requires the use of supercomputers or coarse-grained modeling techniques. One effective approach to reducing the number of particles while preserving the simulation scale is to employ coarse-grained approximations, as implemented in the Martini3 molecular modeling framework [14]. In this approach, between three and ten atoms of an atomistic model are represented by a single bead, significantly reducing the number of pairwise interactions to be calculated and allowing for larger time steps in the simulation. This makes it possible to simulate longer physical times within the same computational cost. There-fore, in this work, the Martini3 package is used for coarse-grained modeling within the GROMACS environment.

An example of the modeled surface in atomistic representation is shown in Fig. 2. In this configuration, the parameters are defined as $d = 10$ nm, $a = 50$ nm, and $h = 10$ nm. The initial structure, generated using a custom Python script, is shown in Fig. 2a, while the same structure after energy minimization is presented in Fig. 2b.

Initially, the polymer structure under consideration was subjected to energy minimization. Subsequently, all degrees of freedom of the polymer atoms were frozen, while all solvent molecules (i.e., water) were as-signed an additional initial uniform velocity corresponding to the overall flow velocity. Then, a coarse-grained molecular dynamics simulation was performed for a duration of 10 ns, during which all molecular forces acting on the polymer atoms were recorded.

The calculated force values were then averaged over time, with sampling performed every nanosecond (resulting in ten measurements). The obtained average value was used as a characteristic quantity, denoted as Fi, representing the mean force exerted by the flow on the surface under the conditions of a specific i-th simulation experiment.

3. RESULTS

The values of the previously defined parameters were investigated within the following ranges:

– the diameter d, chosen as the principal parameter with respect to which the others were varied, ranged from 10 to 50 nm with a step of 10 nm;

– the distance a between adjacent particles varied from d to 5d with a step of d;

– the height h of the particles ranged from 0.5d to 2.5d with a step of 0.5d.

Initially, five experiments were conducted to study the influence of the particle diameter d on the total force acting on the entire surface. In these simulations, the remaining parameters were fixed as follows: $a = 7$d, $h = $ d, $\alpha = 20°$, and the initial macroscopic velocity of water molecules $V = 1$ m/s. As a result, five values of the total acting force were obtained. Although their ab-solute magnitudes are not of direct interest – since they depend strongly on the modeled surface size – their relative ratios are highly informative. Accordingly, among the five obtained force values Fi, the maximum value $F_m = \max(\text{Fi})$ was determined, and all others were normalized to this reference value.

It was established that as the particle diameter increases, the force exerted by the flow on the surface initially increases, but then decreases once the portion of the total surface area occupied by the particle tops exceeds approximately 30–40%. Fig. 3a shows the dependence of the relative force acting on the structured surface on the particle diameter, while Fig. 3b shows the same dependence plotted against the fraction of the surface area covered by the deposited particles.

The next series of experiments investigated the influence of the distance between individual nanoparticles on the force exerted by the flow on the surface. Five experiments were performed in which the distance a varied from d to 5d with a step of d, while the other parameters were kept constant: $d = 20$ nm, $h = $ d, $\alpha = 20°$, $V = 1$ m/s. The obtained dependencies of the acting force on the surface are shown in Fig. 4. Fig. 4a presents the dependence on the distance a, and Fig. 4b shows the dependence on the relative fraction ε_S of the surface area covered by the particles.

Finally, another series of five experiments was conducted to study the influence of particle height h, which varied from 0.5d to 2.5d in increments of 0.5d. The resulting dependence of the normalized force acting on the surface is shown in Fig. 5.

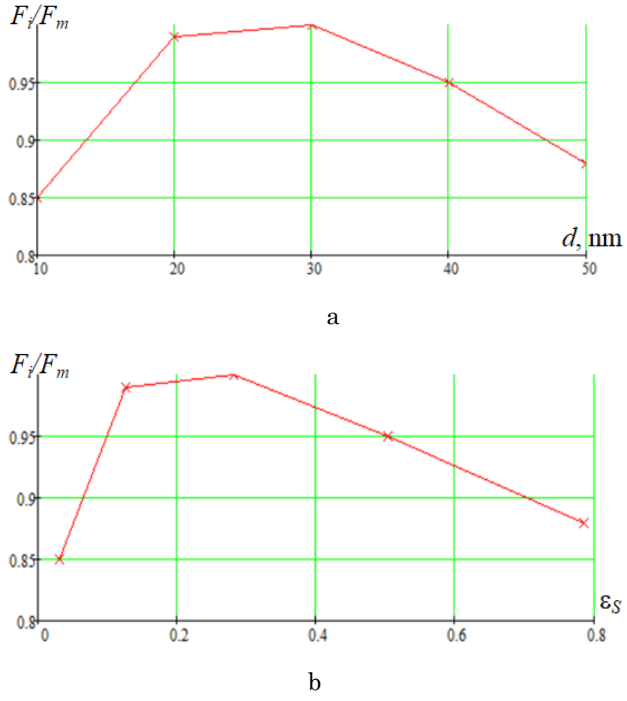


Fig. 3 – Comparative plots of the force acting on the modeled surface from the incident flow: dependence on the diameter of the nanoparticles deposited on the surface (a), dependence on the relative fraction of the surface area covered by nanoparticles (b)

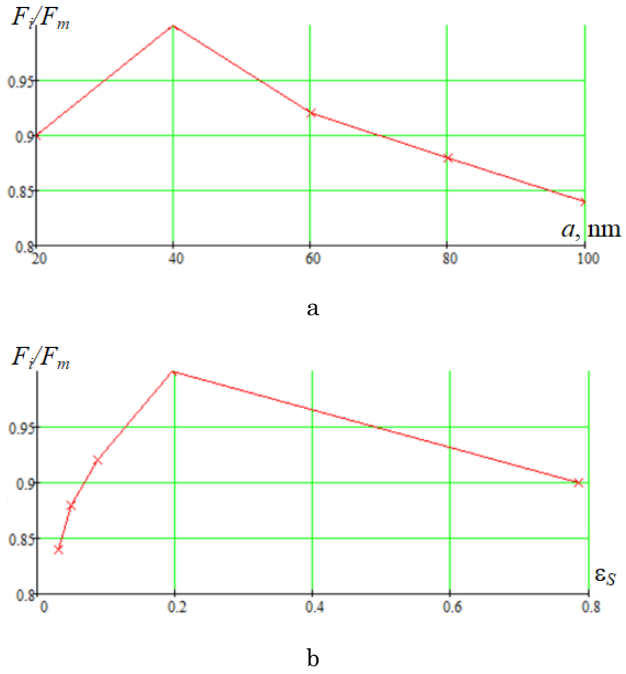


Fig. 4 – Comparative plots of the force acting on the modeled surface from the incident flow: dependence on the distance between nanoparticles deposited on the surface (a), dependence on the relative fraction of the surface area covered by nanoparticles (b)

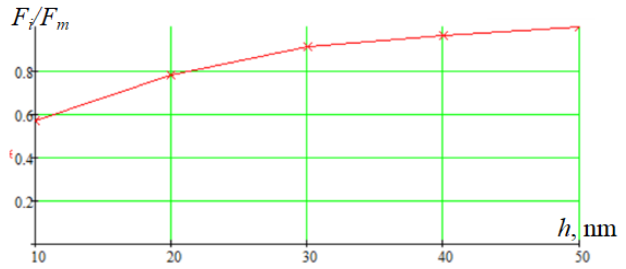


Fig. 5 – Comparative plot of the force acting on the modeled surface from the incident flow as a function of the height of the nanoparticles deposited on the surface

4. DISCUSSION

From the analysis of Fig. 3, it can be observed that a maximum occurs in the range of $d = 20\text{-}30$ nm, corresponding to the case where approximately 10-50 % of the total surface area is covered by deposited nanoparticles. Based on this observation, it can be concluded that particles with a diameter of about 20 nm may pro-vide sufficiently high efficiency, especially when the total area they occupy represents a significant portion of the modeled surface.

Examining Fig. 4, it follows that the maximum flow impact on the surface occurs when the distance between the centers of adjacent particles is approximately twice the particle diameter. It should also be noted that under these conditions, the degree of surface coverage by particles is about 20-30 %, which is generally consistent with the previous series of experiments involving variations in particle diameter.

Finally, Fig. 5 shows an overall direct relationship between the particle height h and the magnitude of the flow-induced force acting on the surface. However, as the particle height increases further, the strength of this dependence gradually weakens. This indicates that excessively increasing the particle height is not practical, and a reasonable intermediate value should be preferred.

It is also important to consider technological constraints. From a fabrication standpoint, the deposition of particles onto a surface (for example, through spraying) is more feasible when the particles have a regular, near-spherical shape, as is typical for nanopowders. Consequently, the particle diameter is likely to be approximately equal to its height, i.e., $h = d$. Under these conditions, the resulting force magnitude reaches about 0.8 of the theoretical maximum value, which is still significant. The absolute maximum, in contrast, is technologically unattainable due to the impracticality of depositing particles with highly elongated shapes and maintaining their strictly perpendicular orientation to the surface.

Therefore, considering realistic technological limitations, in subsequent discussions the deposited particles are assumed to have parameters $d = h = 20$ nm.

5. CONCLUSION

In summary, it can be concluded that the application of a nanocoating to a surface interacting with a liquid flow (for instance, the surface of a turbine blade) leads to a measurable modification of the force exerted on that surface. Under certain technologically feasible conditions – without the need for costly fabrication methods – the magnitude of this force can increase by up to approximately 20%, indicating that the use of such coatings is both effective and practical.

The most favorable performance was achieved when using particles with a size of about 20 nm, which in this study were approximated as cylinders with a diameter and height of 20 nm, arranged at center-to-center distances of around 40 nm. Under these conditions, the fraction of the total surface area covered by deposited particles reaches about 30-40 %, corresponding to the most efficient configuration identified in the simulations.

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Аналіз ефективності нанопокриттів для поверхонь лопаток підводних турбін з вертикальною віссю

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У роботі досліджено потенціал підвищення ефективності підводних турбін з вертикальною віссю шляхом нанесення наноструктурованих покриттів на поверхні лопатей. Запропонований підхід передбачає формування простого періодичного нанопокриття, що складається з рівномірно розподілених циліндричних наночастинок, закріплених на поверхні. Використовуючи моделювання молекулярної динаміки в рамках Gromacs та грубозернистої моделі Martini3, було проаналізовано взаємодію між потоком рідини та наноструктурованими поверхнями. Систематично досліджувався вплив діаметра наночастинок (10-50 нм), відстані між ними (d – 5d) та висоти (0,5d – 2,5d) на загальну гідродинамічну силу, що діє на поверхню на нанорівні. Було розглянуто дві стратегії моделювання: застосування імпульсу початкової швидкості та підтримка постійного потоку за допомогою постійної об'ємної сили. Результати показують, що відносна сила, що діє з боку потоку, сильно залежить від геометричних характеристик нанопокриття. Чіткий максимум спостерігався для частинок діаметром приблизно 20 нм, що відповідає покриттю поверхні близько 30-40 %. Збільшення висоти частинок збільшує передану силу до певної межі, після якої ефект насичується. Технологічні міркування вказують на те, що покриття, утворені шляхом осадження майже сферичних частинок, де $h \approx d$, є найбільш доцільними. За таких реальних умов застосування нанопокриття може збільшити ефективну силу взаємодії – і, таким чином, ефективність перетворення енергії потоку – до 20 %. Ці результати свідчать про те, що наноструктуровані поверхні лопатей можуть бути практичним та економічно ефективним засобом підвищення продуктивності підводних турбінних систем.

Ключові слова: Поверхнева наноструктура, Взаємодія рідина-тверде тіло, Потік води, Молекулярна динаміка, Крупнозернисте моделювання, Ефективність взаємодії.