Simulation the motion of a viscous fluid containing graphene plates in the gap between static and rotating stepped discs

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Abstract. The motion of a viscous fluid containing graphene nanostructures in a thin gap between a stationary stepped stator and a rotating stepped rotor is considered. Dependences are obtained for calculating the parameters of motion of an elementary volume of a viscous liquid. Using the Maple mathematical package, characteristic trajectories of movement of elementary volumes of fluid in the gap are obtained. A similar idea of the movement trajectories of an elementary volume was obtained using computational fluid dynamics using the FlowVision package (TESIS, Russia). The transition from a mathematical description to a computer model makes it possible to take into account changes in the viscosity of a liquid caused by a change in the concentration of graphite in the initial suspension. The use of a computer model opens the way to modeling the mixing of graphene nanostructures with a viscous liquid.

1. Introduction

The main functional purpose of lubricants is to reduce the coefficient of friction between surfaces moving relative to each other and to reduce their wear. The analysis of promising developments and studies reviewed by scientists from different countries and presented in the journal Friction and Wear over the past 35 years is given in the review [1]. The addition of nanoparticles to lubricating oils and greases significantly reduces interfacial friction and increases the load-carrying capacity of parts, which is considered a great potential as lubricating additives. Few-layer and multilayer graphene are very promising nanoaditives for lubricants. The study [2] presents the macrotribological behavior of graphene-containing oil during lubrication of steel / steel contacts. It has been experimentally proven that graphene plates as an additive to the base oil can, especially in the boundary lubrication mode, reduce friction in steel / steel contacts by up to 44%. It was shown that the predominant mechanism for lubricating graphene plates is the formation of a protective tribofilm on the contacting surfaces.

Not only low-layer and multilayer graphene, but also graphene derivatives are used as additives to lubricants. Three-dimensional hierarchical porous graphene as an additive to lithium grease was investigated by measuring the morphology and volume loss of the worn surface in three modes of motion [3]. The results show that the addition of graphene can significantly improve the friction reduction and anti-wear properties of the lubricant and thus results in a smoother wear surface. Specifically, a grease with 0.3 wt% graphene can be reduced by 52.0% and 20.3% in wear volume loss and coefficient of friction, respectively, compared to the original grease.

Interest in few-layer and multi-layer increased after they learned how to obtain these products by liquid-phase shear exfoliation of graphite, i.e. without the use of strong acids. Liquid phase exfoliated graphene sheets were modified by oleic acid and dispersed in lubricant oils as additives [4]. The tribological behaviours of graphene-contained oils were investigated using a four-ball tribometer. The lubricant with optimized graphene concentrations of 0.02–0.06 wt% showed enhanced friction and anti-wear performance, with friction coefficient and wear scar diameter reduced by 17% and 14%, respectively. The titanium
complex grease was prepared by dispersing graphene (GN) with a proper concentration into the titanium complex grease [5]. In order to uniformly disperse it into the base grease, the GN-oil dispersion was prepared; then the GN-oil dispersion was added into the reaction mixture with the weight concentration of GN 0.02, 0.04, 0.06, 0.08, 0.1%; and then, based on the variations of the average friction coefficient (AFC) and wear scar diameter (WSD) with the additive concentrations, the grease containing the optimum concentration of GN was determined carried out with the four-ball tester. It was the titanium complex GN grease that consisted of base grease and GN with the optimum additive concen. When the addition was 0.02 wt% dosage, the AFC of Grease A and B decreased by about 13.8% and 5.0%. When the concentration was 0.06 wt%, the AFC was minimum, being reduced by 21.99% and 21.25% compared with the base greases A and B, respectively. As the amount of GN further increased, the AFC slightly increased. It indicated that the antifriction effect was weakened when the dosage of GN was excessive.

We get graphene directly in oil, which is the basis of the lubricant. The results of our experimental studies showed that the diameter of the wear spot of a lithium complex lubricant for threading from a pipe plant is 50% larger than when using the same lubricant modified with 0.1% multilayer graphene (graphene plates) [6]. Disk devices that use the energy of shear deformations in the gap between the rotating and fixed discs hold great promise for dispersing and homogenizing nanoparticles in a liquid base. For the transition from laboratory to industrial installations, a mathematical model was developed for the movement of a viscous fluid in a small gap between a moving and rotating discs [7]. This model makes it possible to determine the basic geometric and operating parameters of a device for homogenizing viscous liquids, in particular lubricants. Subsequent studies have shown that increasing the homogeneity of the mixture of the initial lubricant and the graphene modifier, it is necessary to increase the path length of this viscous liquid in the gap between the discs. The easiest way to solve this problem is to increase the geometric dimensions of the device, but this is an extensive way. We solved this problem by changing the disk configuration.

2. Simulation object and problem statement
In the previous study [7], we considered the scheme presented in figure 1. In this article, we consider an installation with a stepped rotor, the diagram of which is shown in figure 2.

figure 1. Geometric interpretation of movement in the gap between the disks: front view with a cut (a), top view (b).
The installation contains a cylindrical rotor 1, which is located inside the cylindrical stator 2. The lower plane of the rotor and the bottom of the stator are stepped. Lubricant containing graphite or multilayer graphene is pumped into hole 3. When the rotor rotates, the lubricant passes between the stationary stator and the moving rotor along the gaps 4 and then goes up through the gap 5. In the vertical sections, the gap between the stator and the rotor is 0.1 mm, and in horizontal sections, the gap can be changed by moving the rotor in the vertical direction. Since the speed of movement varies along the height of the gap, it practically changes from zero, near the housing 1, to the peripheral speed of the rotor 2, the lubricant layers are shifted relative to each other, homogenization occurs.

The modeling problem can be formulated as follows: find the velocity of the distribution of a viscous fluid in a stationary mode in the gap between the body and the rotor, as a function of the coordinates of the elementary volume of this fluid. Knowledge of the distribution of velocities allows not only to start modeling the homogenization process, but also to calculate the geometric and operating parameters of the industrial installation to ensure the required mode of motion.

The use of a stepped stator and rotor made it possible, without changing the overall dimensions of the device, to almost double the path of movement of the lubricant in a thin gap between the stationary stator and the rotating rotor. In addition, periodic changes in the direction of movement, during transitions from horizontal to vertical sections and vice versa, not only intensify the homogenization process due to the occurrence of turbulent flows, but also contribute to the exfoliation of graphite or multilayer graphene.

3. Mathematical description of motion

For the installation, the diagram of which is shown in figure 1, we used a cylindrical coordinate system and obtained the following dependences to describe the trajectory of motion of an elementary volume of a lubricant and graphene nanostructures that are in this volume [7]:

\[ r(\tau) = \frac{\sqrt{\pi \cdot h \cdot (V \cdot \tau + r_0^2 \cdot \pi \cdot h)}}{\pi \cdot h} \]  \hspace{1cm} (1)

\[ \varphi(\tau) = \varphi_0 + \frac{\omega \cdot x \cdot \tau}{h} \]  \hspace{1cm} (2)

where \( h \) - gap size (m), \( V \) - volumetric capacity (m³/s), \( \tau \) - current time (s), \( r_0 \) - radius for lubricant hole (m), \( x \) - distance from the considered elementary volume to the stator, m.

It should be especially noted that the change in the angular coordinate (dependence 2) depends on the position of the elementary volume in the gap between the stator and the rotor. Parameter \( X \) can vary from 0 to 1.
For the installation, the diagram of which is shown in figure 2, the stator and rotor are stepped, therefore there are two types of sections with different patterns of viscous fluid movement. The trajectories and nature of movement on horizontal sections can be determined by dependencies (1) and (2), i.e. the movement of elementary volumes is carried out in a spiral. In vertical sections, elementary volumes move along a helical path. It should be especially noted that the pitch of the spiral decreases with distance from the axis of rotation of the rotor, but the helical lines within one section have a constant pitch. The velocity of the elementary volume along the $x$-axis in vertical sections can be calculated using the following relationship:

$$w_x = \frac{V}{\pi(R_s^2 - R_R^2)} \tag{3}$$

With this in mind:

$$x(\tau) = w_x \cdot \tau = \frac{V \cdot \tau}{\pi(R_s^2 - R_R^2)} \tag{4}$$

$R_s$ – the radius of the stator in the section $i$, $R_R$ – the radius of the rotor in the section.

The angular coordinate can be calculated as follows:

$$\phi_i(\tau) = \phi_{0i} + \frac{\omega \cdot (R_s - r) \cdot \tau}{(R_s^2 - R_R^2)} \tag{5}$$

$\phi_{0i}$ – the angular coordinate at which the elementary volume began to move in the vertical section (the numbering of the vertical sections starts from the rotor axis), $r$ - current radius at which the elementary volume is located in the vertical section.

4. Results and discussion

Using solutions (1, 2) and (4, 5), it is easy to obtain the characteristic trajectories of the elementary volumes of a viscous fluid and graphene particles that are in these volumes, in the gap between a stationary step stator and a rotating step rotor with different flow characteristics and device geometry. In addition, the residence time of these elementary volumes in the gap and the path length can be calculated. Figure 3 shows a typical trajectory of movement of an elementary volume. This trajectory is calculated at a productivity $V = 0.1 \times 10^{-6}$ m$^3$/s, an angular rotor speed $\omega = 52.36$ rad/s (500 rpm) and geometric parameters that are shown in Figure 2, i.e. we used the same parameters as in the previous study [7]. It should be noted that the path length of the elementary volume of the lubricant in the gap increased by about 2 times. The movement of a viscous fluid in a small gap between a stationary stepped stator and a rotating stepped rotor was modeled by computational fluid dynamics using the FlowVision package (TESIS, Russia). For this, a three-dimensional model was imported into the program, which describes the "liquid region". In addition, the parameters corresponding to Figure 2 were corrected. Using a laminar fluid model and setting the boundary conditions at the inlet and outlet ($V = 0.1 \times 10^{-4}$ m$^3$/s) and the boundary condition of the wall on a stationary and rotating wall (stator and rotor), the velocity and pressure fields were calculated and the trajectories of the elementary volume were visualized. Figure 3 shows that in the horizontal sections the pitch between the turns decreases with increasing distance from the axis of rotation of the rotor, and in the vertical sections the pitch of the spiral within the boundaries of each section remains constant. Experimental studies on a laboratory setup with a rotor diameter of 62 mm and speeds from 300 to 1500 rpm showed satisfactory convergence of the calculated and experimental values. The choice of optimal geometric and operating parameters can be done after experimental studies of the influence of these parameters on the performance characteristics of the finished product. If we consider the process of modifying lubricants with graphene nanostructures, then the main performance characteristics are the coefficient of friction and wear.
5. Conclusion
A mathematical description of the motion of a viscous fluid with graphene nanostructures in the gap between a stationary stepped stator and a rotating stepped rotor has been developed. Using the Maple mathematical package, characteristic trajectories of movement of elementary volumes of fluid in the gap are obtained. A similar idea of the movement trajectories of an elementary volume was obtained using computational fluid dynamics using the FlowVision package (TESIS, Russia). The transition from a mathematical description to a computer model makes it possible to take into account changes in the viscosity of a liquid caused by a change in the concentration of graphite in the initial suspension. The use of a computer model opens the way to modeling the mixing of graphene nanostructures with a viscous liquid.

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