Simulation of the oil film thickness on a friction surface in the presence of fullerene compositions in the lubricant

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Abstract. The paper contains theoretical studies of the oil film formation on a friction surface in the presence of fullerene solutions in a lubricant. The mathematical model is developed on the basis of the interaction between electrically active heterogeneous finely dispersed systems at the interface between the friction surface and the lubricating medium and is described by the Poisson differential equation. The role of the friction surface on the formation of clusters and micelles in an adsorbed film of the lubricant near the friction surface is established. It is shown that in the stress-strain state of triboelement material surface layers, the friction surface acts as an “electrostatic field generator”. Expressions are obtained for the simulation of the oil film thickness in the presence of fullerenes in the base lubricant. Based on the simulation results, the most significant factors in the formation of the oil film thickness have been established: these are the electric field strengths of the friction surface and the base lubricating medium; the load on the tribosystem; the temperature, and dynamic viscosity of the lubricating medium.

1. Introduction

Today, the use of nanocarbon additives and supplements (C₆₀ fullerenes) is of great interest [1]. The work [2–4] presents the results of studies devoted to the effect of fullerene additives to lubricants on the processes of friction and wear of metals under boundary lubrication conditions; a conclusion is made here about the prospects of using such additives.

The complexity of this problem is that it is impossible to study the mechanisms of interaction between active elements of a lubricating medium, for example, fullerenes in the process of friction and their interaction with the friction surface. At the same time, during the tribosystem operation under the action of plastic and elastic deformation of a surface layer roughness and material, the friction surface acts as an “electrostatic field generator”, which affects the ordering of the thin oil film structure and determines the film thickness.

Electrically active dispersed systems with a well-developed specific surface, which include clusters and micelles, particularly fullerene molecules, are one of the promising classes of modern materials. These materials will soon be used in the development of new lubricant compositions. The complexity of the structure of dispersed nanomaterial-based systems, as well as the presence of local inhomogeneities there determine the lack of an established understanding of the mechanism for reducing wear and friction losses in tribosystems where fullerenes are used in lubricants. In the
presence of numerous interfaces in these complex systems, the total effect of interphase interactions becomes especially strong and is decisive for the generation of intrinsic electric fields. This interaction leads to the appearance of electrical forces, and, consequently, to the electrostatic field gradient at the friction surface.

2. Analysis of recent studies and publications
The analysis of the works devoted to the use of fullerenes as additives to lubricants made it possible to conclude that fullerenes are not dispersed in all technical oils, both mineral and synthetic [1, 2]. However, fullerenes are well dispersed by volume in vegetable oils, especially high oleic oils [6]. Therefore, using this phenomenon, it is possible to preliminarily disperse fullerenes in a high oleic vegetable oil, for example, rapeseed one, and then introduce this composition into a lubricant. Thus, it is possible to realize the mechanism of micelle formation near the electrostatically charged friction surface, which will allow the creation of strong surface layers.

In [5, 6], theoretical studies of the formation of an oil film on the friction surface when fullerenes are introduced into vegetable oil followed by their introduction into a lubricant have been carried out. The mathematical model is developed on the basis of the interaction between electrically active heterogeneous fine-dispersed systems at the interface between the friction surface and the lubricating medium and is described by the Poisson differential equation. The relationship between the electrostatic field on the friction surface and the electric field in the volume of the liquid is shown, as well as the role of the friction surface on the formation of clusters and micelles in a lubricant film at the friction surface. It was found that under the stress-strain state in surface layers, the friction surface acts as an “electrostatic field generator”, which affects the formation of an electric field in the volume of an oil film with a micellar structure [9]. Expressions for calculating the strength of the total electric field in the system “friction surface + lubricant” are obtained.

3. Statement of the objective and tasks of the study
The purpose of this work is to carry out theoretical studies of the oil film thickness formation on the friction surface in the presence of fullerene compositions in the lubricant.

The structure of a mathematical model for the thickness formation of a lubricating film containing fullerenes on the friction surface of a tribosystem is described in [7, 8] and contains:
- Simulation of the electrostatic field strength of the friction surface during the tribosystem operation, which can be expressed as surface energy with dimension in J / m², or as surface charge density with dimension in C / m²;
- Simulation of the electric field strength within the lubricant volume, which is under the influence of the force field of the friction surface, and which contains fullerenes and other molecules of surfactants;
- Simulation of the oil film thickness formation on the friction surface of the tribosystem, which is formed due to the “stitching” of spatial aggregates, micelles and clusters, into a volumetric structure resembling a honeycomb structure.

The formation of "stitched" structures on the friction surface leads to a change in the arithmetic mean deviation of the profile points Ra, μm, and the average roughness width along the midline of the profile Sm, mm, for newly formed friction surfaces.

Determination of the dependences of the Ra decrease with a simultaneous increase Sm with a change in the oil film thickness allows reducing the wear rate and lowering friction losses during the operation of tribosystems.

4. Development of mathematical model
The most convenient method for determining the electric field strength is to solve the differential equation for the potential, which is presented in [7]:

\[ \frac{\partial^2 \phi}{\partial z^2} = -\frac{\rho}{\varepsilon \varepsilon_0} = -(E_n + E_k + E_m) \]

where \( \phi \) is the electric potential, V; \( z \) is the coordinate perpendicular to the friction surface; \( \rho \) is Volumetric charge density; \( \sigma \) is surface charge density, C / m²; \( \varepsilon \) is relative dielectric constant of the
lubricating medium; \( \varepsilon_0 \) is a dielectric constant equal to \( 8.85 \cdot 10^{-12} \text{ C/V \cdot m} \) or \( \text{F/m} \); \( E_n \) is the strength of the electrostatic field created by the friction surface during operation, \( \text{V/m} \); \( E_p \) is the strength of the electrostatic field within the lubricating film volume due to the formation of clusters from fullerenes, \( \text{V/m} \); \( E_m \) is the intensity of the electrostatic field within the lubricating film volume due to the formation of micelles from fullerenes, \( \text{V/m} \).

The first term on the right-hand side of equation (1) determines the intensity of the electrostatic field created by the friction surface during operation:

\[
E_n = \frac{\sigma}{2\varepsilon_0}, \text{ V/m,} \tag{2}
\]

where \( \sigma \) is the surface charge density, \( \text{C/m}^2 \), which is determined by the formulas given in [7].

The second term on the right-hand side of equation (1) determines the electric field strength in the lubricating film volume due to the formation of clusters from fullerenes:

\[
E_k = \frac{n_k P_k}{4\pi\varepsilon_0 d_k^3}, \text{ V/m,} \tag{3}
\]

where \( n_k \) is the number of clusters per unit volume of the base lubricant, pcs.; \( P_k \) is the dipole moment of clusters, with dimension in \( \text{Kl \cdot m} \); \( d_k \) is the average distance between clusters and the friction surface equal to the average size (diameter) of the cluster, with dimension in m (metres).

The work [7] presents formulas for determining the value depending on the change in the concentration of fullerenes, the temperature of the lubricating medium, and the electrostatic field strength magnitude on the friction surface.

The third term on the right-hand side of equation (1) determines the electric field strength within the lubricating film volume due to the formation of micelles, where a fullerene molecule or a cluster of fullerenes acts as a nucleus, which surrounds attached molecules of a high-molecular acid (oleic, stearic, etc.) ... Such acids act as a "solvent" for fullerenes. The expression for determining the electric field magnitude due to the formation of micelles is written in the form:

\[
E_m = \frac{n_m P_m}{4\pi\varepsilon_0 d_m^3}, \text{ V/m,} \tag{4}
\]

where \( n_m \) is the number of micelles per unit volume of the base lubricant, pcs.; \( P_m \) is the dipole moment of the micelle, \( \text{C \cdot m} \); \( d_m \) is the average distance between the micelle and the friction surface, equal to the average size (diameter) of the micelle, with dimension in m.

The work [7] presents formulas for determining the value \( E_m \) depending on the change in the concentration of micelles, the temperature of the lubricating medium, and the electrostatic field strength magnitude on the friction surface.

During the functioning of the tribosystem, the process of cluster and micelle formation, as well as their destruction due to the influence of temperature, as well as the load and sliding speed, can occur simultaneously; therefore, the total electric field of the lubricating medium is determined as the sum:

\[
E_g = E_k + E_m, \text{ V/m,} \tag{5}
\]

Applying the dimensional analysis method, which is widely used in the theory of similarity and modelling, as well as experimental data, it is possible to obtain an expression for determining the thickness of the lubricating film, which will be formed on the friction surface under the influence of the electric force fields on the friction surface and in the liquid:

\[
h = \frac{\mu(T) \cdot A_{mp} \cdot \nu_{ekz} \left( E_n + E_{\infty} \right)}{N \sqrt{E_n^2 + E_g^2}}, \text{ m,} \tag{6}
\]
where \( h \) is the lubricating film thickness, m; \( \mu(T) \) is the function of changing the dynamic viscosity of the base lubricant medium depending on temperature, Pa \( \cdot \) s; \( A_{nm} \) is the actual friction area, which is the sum of the friction areas of all patches of actual contact, with dimension in m\(^2\), is determined by the formulas given in the work [10]; \( \nu_{ccl} \) is sliding speed, m/s; \( N \) is the tribosystem load, N.

The operating temperature in the volume of the oil film \( T \) is determined by the expression:

\[
T = T_{oc} \cdot \exp\left(W_{mp} \cdot f\right), \degree C,
\]

where \( T_{oc} \) is the ambient temperature, \degree C; \( W_{mp} \) is the rate of work of dissipation in the tribosystem, J/s; it is determined by the method described in the work [10]; \( f \) is the coefficient of friction; a dimensionless quantity, which is determined by the method described in the work [10].

The function of changing the dynamic viscosity of the lubricating medium with a change in temperature is determined by the expression:

\[
\mu = \mu_0 \cdot \exp\left(-\alpha(T - T_0)\right), \text{Pa s},
\]

where \( \mu_0 \) is the dynamic viscosity of the lubricant at 100 \degree C, Pa \( \cdot \) s; \( \alpha \) is the piezo coefficient equal to 0.013; \( T \) is the working temperature determined by the formula (7), \degree C; \( T_0 \) is the temperature at which \( \mu_0 \) is determined, i.e. equal to 100 \degree C.

The result of the \( \mu(T) \) change obtained using formulas (7) and (8) is substituted into expression (6) to simulate the change in the thickness of the lubricating film \( h \).

5. The results of the calculation and their discussion

The results of simulation of the change in the oil film thickness on the friction surface depending on the strength of the electric fields of a friction surface and a liquid are shown in figure. 1. When analysing the dependences, it can be concluded that the magnitude of the electrostatic field strength on the surface \( E_n \) is a more significant factor than the magnitude of the electric field strength of the liquid \( E_g \). As follows from figure. 1, at small values of \( E_n = 2.5 \times 10^6 \) V/m, the film is of one oleic acid molecule thickness \( h = (1 - 7) \times 10^{-11} \) m. With an increase in \( E_n = 7.5 \times 10^6 \) V/m, the film thickness increases to \( h = 1 \times 10^{-6} \) m. The obtained simulation results confirm that the friction surface, being a "generator of an electrostatic field", is a more significant factor in the formation of an oil film on the friction surface.

![Figure 1](image1.png)  
**Figure 1.** Dependences of the change in the oil film thickness on the electric field strengths on a friction surface and in a liquid.

The degree of influence of the operating temperature \( T \) \degree C in the oil film volume, as well as the dynamic viscosity of the base lubricant \( \mu \), Pa \( \cdot \) s on the lubricating film thickness depending on the total strength of the electric fields \( E=E_p+E_g \) is shown in Figure 2 and Figure 3.

![Figure 2](image2.png)  
**Figure 2.** Dependences of the change in the lubricating film thickness on the magnitude of the total strength of electric fields and on operating temperature.
Figure 3. Dependences of the change in the lubricating film thickness on the total value of the electric field strengths and the dynamic viscosity of the base oil.

When analysing the dependences, it can be concluded that a change in temperature from $T = 80 \, ^\circ C$ to $T = 160 \, ^\circ C$ leads to a decrease in the film thickness from $h = 4.5 \cdot 10^{-7} \, m$ to $h = 2.5 \cdot 10^{-7} \, m$. Similar dependences were obtained when changing the dynamic viscosity of the base oil, figure. 3.

The degree of tribosystem load influence on the lubricating film thickness is shown in figure. 4. It follows from the dependences that an increase in the load $N$, significantly reduces the oil film thickness.

As follows from the obtained theoretical dependencies, the most significant factors in the formation of the oil film thickness are: the electric field strengths on a friction surface and in a liquid; load on the tribosystem; temperature and dynamic viscosity of the lubricant.

6. Conclusions

It is shown that the electrical interaction in a lubricating medium of clusters and micelles, which include fullerenes, is described by the Poisson differential equation and its solution contains three components: the electrostatic field strength on the friction surface; the electric field strength in the volume of the liquid due to the formation of clusters; electric field strength in the volume of the liquid due to the formation of micelles.

The friction surface role in the formation of clusters and micelles in an adsorbed film of a lubricant near the friction surface is established. It is shown that in the stress-strain state of the surface layers of triboelement materials, the friction surface acts as a "generator of an electrostatic force field". Expressions are obtained for simulation of the oil film thickness in the presence of fullerenes in the base lubricant.

Based on the simulating results, the most significant factors in the formation of the oil film thickness were established: these are electric field strengths on the friction surface and in the base lubricating medium; the tribosystem load, the temperature and dynamic viscosity of the lubricant.

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