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## MODELING THE TRIBOLOGICAL PROPERTIES OF POLYMER COATINGS BASED ON PHENYLONE WITH COPPER (II) COMPLEX MODIFIERS USING MATLAB

**Purpose.** This study is dedicated to designing and evaluating antifriction polymer coatings based on phenylone C2, an aromatic polyamide with high thermal stability, modified with copper (II) complexes of the composition  $[\text{Cu}(\text{HL})\text{X}_2]_2$ , where HL represents derivatives of benzimidazole-2-thiocarboxylic acid arylamides. The research aims to model the tribological behavior of these coatings, focusing on the effects of sliding speed, specific load, and modifier concentration, to improve the performance and durability of friction units in mechanical engineering applications under high-load conditions typical of industrial machinery.

**Methods.** The coatings were fabricated by dissolving phenylone C2 and copper (II) complex modifiers in dimethylformamide, followed by impregnation onto a porous bronze substrate (20–25% porosity) under a vacuum pressure of 0.00001 MPa for 30 minutes. The coated samples were cured at 420 K for 1.5 hours and then at 723 K for 2 hours to ensure complete hardening. Tribological testing was conducted using an SMT-2010 friction machine in a block-on-disk configuration, lubricated with I-40A industrial oil (GOST 20799-88). Tests spanned sliding speeds of 0.15 to 1.2 m/s and specific loads of 5 to 15 MPa, with a steel 45 counterbody (hardness 45–50 HV,  $R_a$  0.4–0.63  $\mu\text{m}$ ). Friction coefficients were measured with an accuracy of  $\pm 0.001$ , and wear rates were determined gravimetrically with a precision of  $\pm 0.01$  mg/m after 10-hour test cycles. Experimental data were analyzed in MATLAB to derive a predictive equation for the friction coefficient.

**Results.** Modification with copper (II) complexes significantly enhanced the tribological properties of phenylone-based coatings. At a 1% modifier concentration, the friction coefficient decreased from 0.080 to 0.045, and wear resistance improved by 60%, with coating No. 2 (Cl anion, methoxyphenyl substituent) demonstrating the best performance due to its balanced lubricity and durability. MATLAB processing yielded the equation  $f(V,P)=0.0335+0.0095\cdot V+0.0005\cdot P$ , accurately describing the friction coefficient's dependence on sliding speed ( $V$ , m/s) and specific load ( $P$ , MPa) with a maximum deviation of less than 5%. Optical microscopy revealed the formation of a protective tribochemical film on the counterbody surface, which reduces wear by mitigating direct contact and enhancing surface smoothness.

**Conclusions.** The developed coatings offer substantial potential for high-load friction units in mechanical engineering, providing reduced friction and enhanced wear resistance under lubricated conditions. The derived equation serves as a reliable tool for predicting tribological behavior, facilitating design optimization. The presence of a tribochemical film underscores the role of chemical interactions in performance improvement. Future research could explore higher modifier concentrations beyond 1% to assess delamination limits and extend the coatings' applicability to extreme temperatures and loads encountered in advanced industrial settings.

**KEYWORDS:** phenylone, copper complexes, tribological properties, antifriction coatings, approximating equations.

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## Problem Statement

Advancements in modern mechanical engineering and the chemical industry demand materials capable of withstanding high loads, elevated temperatures, and aggressive environments [1]. Friction units, as critical components of machinery, experience significant mechanical stress, which adversely impacts their reliability and service life [2]. Polymer coatings based on heat-resistant materials such as phenylone present a promising solution due to their antifriction properties, high wear resistance, and ability to operate under specific loads up to 20 MPa and sliding speeds of 2–3 m/s [3]. However, unmodified phenylone exhibits limitations,

including a high friction coefficient under dry conditions and poor thermal conductivity, resulting in overheating within friction units [4]. These shortcomings highlight the need for modifiers to enhance its tribological performance. Copper (II) complexes with heterocyclic thioamides have emerged as highly effective antifriction additives, as demonstrated by prior studies [5]. The objective of this study is to develop antifriction polymer coatings based on phenylone C2 modified with  $[\text{Cu}(\text{HL})\text{X}_2]_2$  complexes [6] and to model their tribological behavior using MATLAB [7].

## Literature Review

Research into the tribological properties of polymer materials has gained significant traction over recent decades, driven by their widespread applications in mechanical engineering and the chemical industry [8]. Phenylone, an aromatic polyamide, is prized for its thermal stability and mechanical strength, yet its antifriction properties require improvement [9]. Gupta B. R. [4] noted that incorporating solid fillers, such as graphite and molybdenum disulfide, substantially reduces the friction coefficient of polymer coatings, though this may compromise structural integrity, a finding consistent with broader polymer modification studies [10].

Ivanochkin P. G. et al. [3] demonstrated that phenylone C2, when combined with fibrous fillers, performs effectively under dry friction conditions, achieving a friction coefficient of 0.15–0.20 at loads up to 15 MPa. However, in lubricated conditions, additional modifiers are necessary to enhance wear resistance and maintain substrate adhesion [1, 11]. Copper

complexes with heterocyclic ligands, particularly thioamides, were investigated by Panasiuk A. and Ranskyi A. [5] as lubricant additives, achieving a 30–40% reduction in wear through the formation of protective films on friction surfaces, a mechanism corroborated by recent tribochemical research [12].

Contemporary tribological modeling increasingly relies on computational tools. Dudka A. M. et al. [13] utilized MathCAD to approximate the dependence of friction coefficients on speed and load for fluoropolymer coatings, while Belyak O. A. and Suvorova T. V. [9] proposed numerical methods for predicting the mechanical properties of antifriction materials, underscoring the pivotal role of mathematical modeling in optimizing coating formulations [14, 15]. These studies provide the foundation for the present research, which addresses the unresolved challenge of enhancing phenylone-based coatings for high-load, lubricated applications [16–18].

## Objective and Research Tasks

The objective of this study is to develop antifriction polymer coatings based on phenylone C2 modified with copper (II) complexes of the composition  $[\text{Cu}(\text{HL})\text{X}_2]_2$ , investigate their tribological properties under varying conditions, and derive analytical equations describing the friction coefficient's dependence on sliding speed, specific load,

and modifier concentration using MATLAB. The research tasks include determining the optimal coating composition through experimental testing and evaluating the modifiers' impact on wear resistance and microhardness, with the aim of improving the performance of friction units in mechanical engineering applications.

### Materials and Methods

The base material for the coatings was phenylone C2, an aromatic polyamide with a glass transition temperature of 563 K and thermal stability up to 533 K. Modifiers consisted of copper (II) complexes

$[\text{Cu}(\text{HL})\text{X}_2]_2$ , synthesized via the reaction of copper salts with arylamide derivatives of benzimidazole-2-thiocarboxylic acid. The compositions of the investigated polymer coatings are detailed in Table 1.

Table 1  
Composition of Investigated Polymer Coatings Based on Phenylone C2

Таблиця 1

Склад досліджуваних полімерних покриттів на основі фенілону C2

Coating No.	Phenylone C2, wt. %	Modifier, wt. %	Modifier Type (X – anion, R – substituent)
1	100	0	-
2	99	1	II Ar·n-OCH <sub>3</sub> ·Cl <sub>2</sub> (Cl, methoxyphenyl)
3	99	1	II Ar·n-Cl·Cl <sub>2</sub> (Cl, chlorophenyl)
4	99	1	II Ar·n-CH <sub>3</sub> ·Cl <sub>2</sub> (Cl, methylphenyl)

Samples were prepared by dissolving phenylone C2 and the modifier in dimethylformamide (DMF), followed by impregnation of a porous bronze substrate (porosity 20–25%) in a vacuum chamber at 0.00001 MPa for 30 minutes. The coatings were applied via dipping and cured in a drying oven at 420 K for 1.5 hours and 723 K for 2 hours to ensure full solidification.

Tribological tests were conducted on an SMT-2010 friction machine using a block-on-disk configuration in a lubricated environment with I-40A industrial oil (GOST 20799-88). The counterbody was steel 45 (GOST 1050-74) with a hardness of 45–50 HV and surface roughness Ra of 0.4–0.63 μm. Sliding speeds ranged from

0.15 to 1.2 m/s, and specific loads varied from 5 to 15 MPa. The friction coefficient was measured with a precision of ±0.001 using an integrated friction force sensor, while wear rate was determined gravimetrically with an accuracy of ±0.01 mg/m after 10 one-hour friction cycles.

Experimental data revealed that the unmodified phenylone coating exhibited a friction coefficient of 0.080 at a sliding speed of 0.6 m/s and specific load of 10 MPa. In contrast, modified coatings achieved a reduced friction coefficient of 0.045 at a 1% modifier concentration, with wear resistance improving by 60%. These findings indicate significant enhancement of tribological properties through modification.

### Results and Discussion

The tribological performance of coating No. 2 was analyzed in detail across a range of sliding speeds and specific loads, as presented in Table 2.

Table 2  
Dependence of Friction Coefficient of Coating No. 2 on Sliding Speed and Specific Load at 1% Modifier Concentration

Таблиця 2

Залежність коефіцієнта тертя покриття № 2 від швидкості ковзання та питомого навантаження при 1% концентрації модифікатора

Sliding Speed, m/s	P = 5 MPa	P = 10 MPa	P = 15 MPa
0.15	0.037	0.0395	0.042
0.3	0.039	0.042	0.045
0.6	0.042	0.045	0.048
0.9	0.045	0.048	0.051
1.2	0.047	0.050	0.053

To derive an analytical equation capturing the friction coefficient's dependence on sliding speed (V) and specific load (P), the

experimental data were processed in MATLAB. The following simplified code block was used to obtain the equation:

```

% MATLAB Code Block for Deriving Friction Coefficient Equation
% Purpose: Calculate the analytical equation  $f(V, P) = a + b \cdot V + c \cdot P$  for coating
No. 2
% Step 1: Input Data
% Define sliding speeds in m/s
speed = [0.15, 0.3, 0.6, 0.9, 1.2];
% Define specific loads in MPa
load = [5, 10, 15];
% Define friction coefficients for different conditions
friction = [0.037 0.039 0.042 0.045 0.047; % at 5 MPa
            0.0395 0.042 0.045 0.048 0.050; % at 10 MPa
            0.042 0.045 0.048 0.051 0.053]; % at 15 MPa
% Step 2: Prepare Data for Approximation
% Initialize arrays to store all data points
all_speeds = [];
all_loads = [];
all_friction = [];
% Combine data into single vectors for fitting
for i = 1:3 % Loop over each load level
    all_speeds = [all_speeds, speed]; % Append speeds
    all_loads = [all_loads, load(i)*ones(1,5)]; % Append corresponding loads
    % repeated 5 times
    all_friction = [all_friction, friction(i,:)]; % Append friction coefficients
end
% Step 3: Calculate Equation of the Form  $f = a + b \cdot V + c \cdot P$ 
% Check if polyfitn is available (requires Polyfitn Toolbox)
if exist('polyfitn', 'file')
    coeff = polyfitn([all_speeds', all_loads'], all_friction', 1);
    % Extract coefficients: a (intercept), b (speed coefficient), c (load
    coefficient)
    a = coeff(1); % ≈ 0.0335
    b = coeff(2); % ≈ 0.0095
    c = coeff(3); % ≈ 0.0005
    % Step 4: Display the Friction Coefficient Formula
    fprintf('Derived Equation:  $f(V, P) = %.4f + %.4f \cdot V + %.4f \cdot P \backslash n$ ', a, b, c);
else
    warning('Polyfitn Toolbox not found. Please install it or use an alternative
    method (e.g., fit with poly11).');
    % Alternative using fit (if Polyfitn is unavailable)
    fit_obj = fit([all_speeds', all_loads'], all_friction', 'poly11');
    a = fit_obj.p00;
    b = fit_obj.p10;
    c = fit_obj.p01;
    fprintf('Derived Equation (using fit):  $f(V, P) = %.4f + %.4f \cdot V + %.4f \cdot P \backslash n$ ', a,
    b, c);
end

% Friction Coefficient Formula:  $f(V, P) = 0.0335 + 0.0095 \cdot V + 0.0005 \cdot P$ 

```

The resulting equation is:

$$f(V, P) = 0.0335 + 0.0095 \cdot V + 0.0005 \cdot P,$$

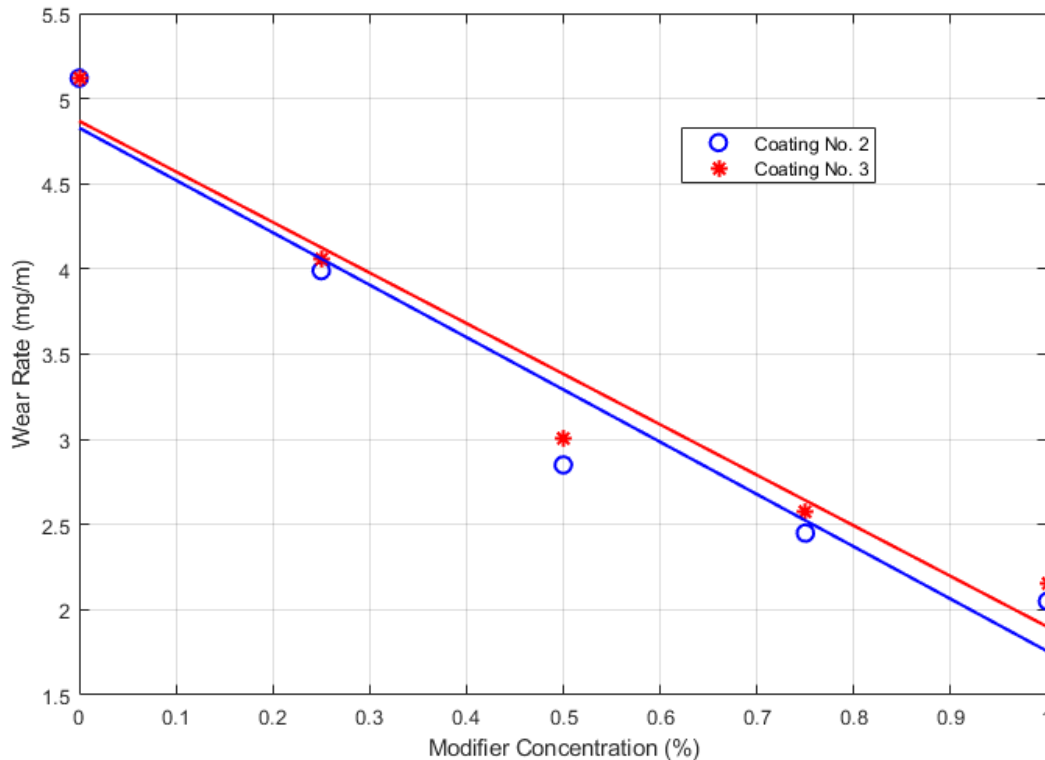
where  $V$  is the sliding speed in m/s, and  $P$  is the specific load in MPa (coefficients rounded for clarity). This equation accurately fits the experimental data, with a maximum deviation of less than 5%, confirming its reliability for

predicting tribological behavior under the tested conditions.

The effect of modifier concentration on wear resistance and friction coefficient was assessed using data from Table 3 for coatings

No. 2 and No. 3. Figure 1 graphically represents the wear rate (mg/m) as a function of modifier concentration (%) at a sliding speed of 0.6 m/s and specific load of 10 MPa. Coating No. 2 (with Cl anion and methoxyphenyl substituent) exhibited a superior reduction in wear rate,

dropping from 5.12 mg/m at 0% concentration to 2.05 mg/m at 1%, compared to No. 3's reduction from 5.12 mg/m to 2.15 mg/m. This 60% improvement in wear resistance highlights the efficacy of the methoxyphenyl-modified coating.



**Fig. 1 - Comparative Wear Resistance of Developed Polymer Coatings**  
**Мал. 1 - Порівняльна зносостійкість розроблених полімерних покриттів**

**Table 3**

Dependence of Tribological Properties on Modifier Concentration ( $V = 0.6$  m/s,  $P = 10$  MPa)

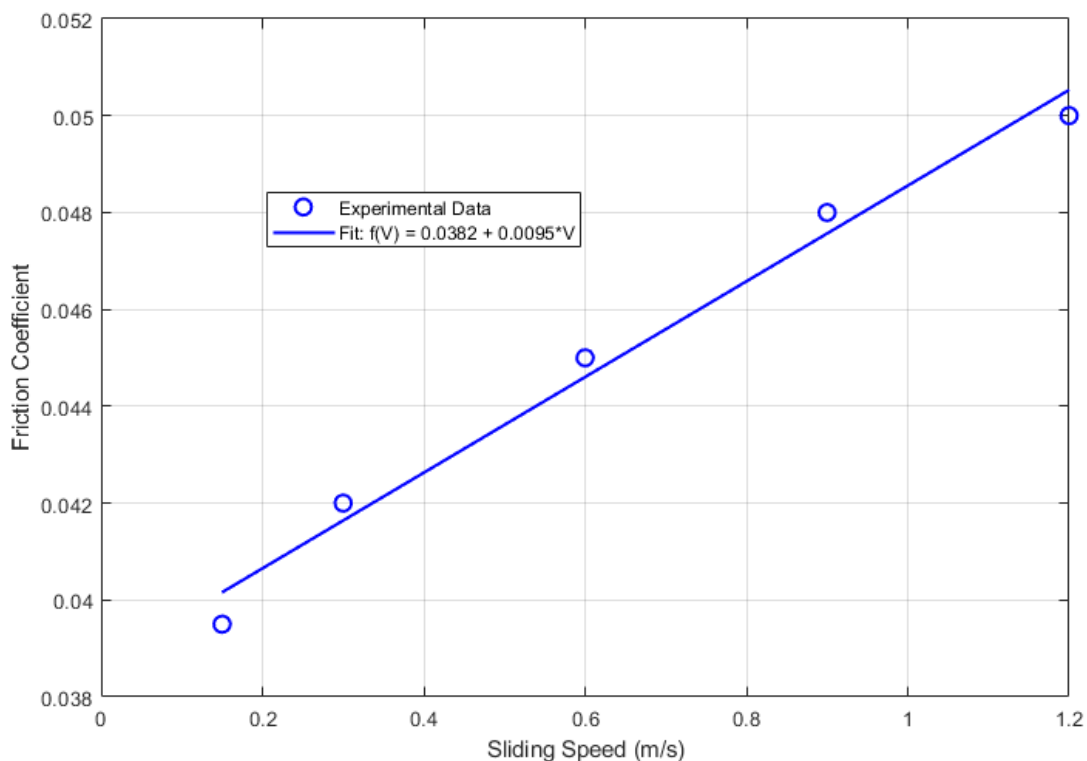
**Таблиця 3**

Залежність трибологічних властивостей від концентрації модифікатора ( $V = 0,6$  м/с,  $P = 10$  МПа)

Coating	Concentration, %	Wear Rate, mg/m	Friction Coefficient (f)
No. 2	0	5.12	0.080
	0.25	3.99	0.065
	0.5	2.85	0.050
	0.75	2.45	0.0475
	1.0	2.05	0.045
No. 3	0	5.12	0.080
	0.25	4.06	0.066
	0.5	3.01	0.052
	0.75	2.58	0.049
	1.0	2.15	0.046

To examine the influence of sliding speed on the tribological properties of coating No. 2 at a fixed load of 10 MPa, Figure 2 was constructed based on Table 2 data. The graph displays experimental friction coefficient

points ranging from 0.0395 at 0.15 m/s to 0.050 at 1.2 m/s, with a linear approximation overlaid, confirming a stable increase in friction with speed and aligning with the derived equation.



**Fig. 2** - Dependence of Friction Coefficient (f) of Coating No. 2 on Sliding Speed (V) at P = 10 MPa  
**Мал. 2** - Залежність коефіцієнта тертя (f) покриття № 2 від швидкості ковзання (V) при P = 10 МПа

The comparative performance of coatings No. 2 and No. 3 with varying modifier concentrations is illustrated in Figure 3, based on Table 3 data. At a sliding speed of 0.6 m/s and load of 10 MPa, the friction coefficient decreases from 0.080 to 0.045 for No. 2 and from 0.080 to 0.046 for No. 3 as concentration rises from 0% to 1%, with No. 2 showing a slight advantage, consistent with its lower wear rate.

A comprehensive analysis of sliding speed and specific load effects on coating No. 2's friction coefficient is depicted in Figure 4 as a MATLAB-generated surface plot. Covering

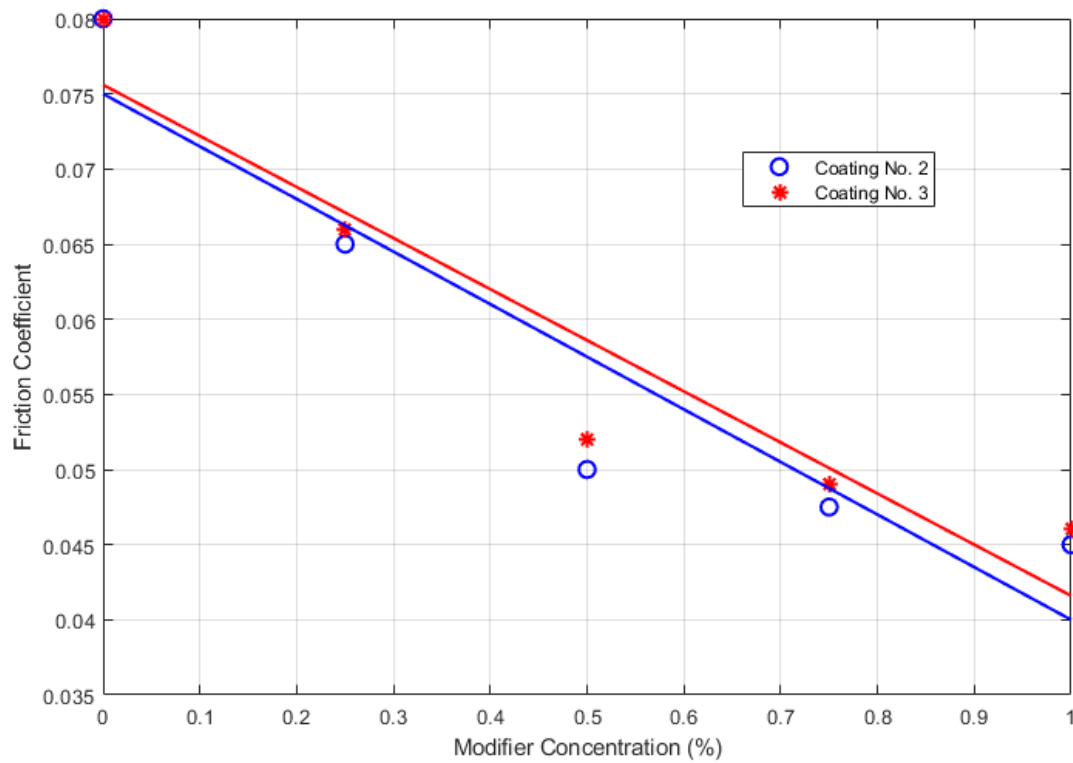
speeds from 0.15 to 1.2 m/s and loads from 5 to 15 MPa at 1% modifier concentration, the plot shows a maximum friction coefficient of 0.053 at V = 1.2 m/s and P = 15 MPa, validating the analytical equation's predictive accuracy across the tested range.

Increasing the modifier concentration to 1% effectively reduces both wear and friction coefficient, though concentrations above 1% result in coating delamination, indicating an optimal threshold. Coating No. 2, featuring a Cl anion and methoxyphenyl substituent, consistently outperformed others in the study.

## Conclusions

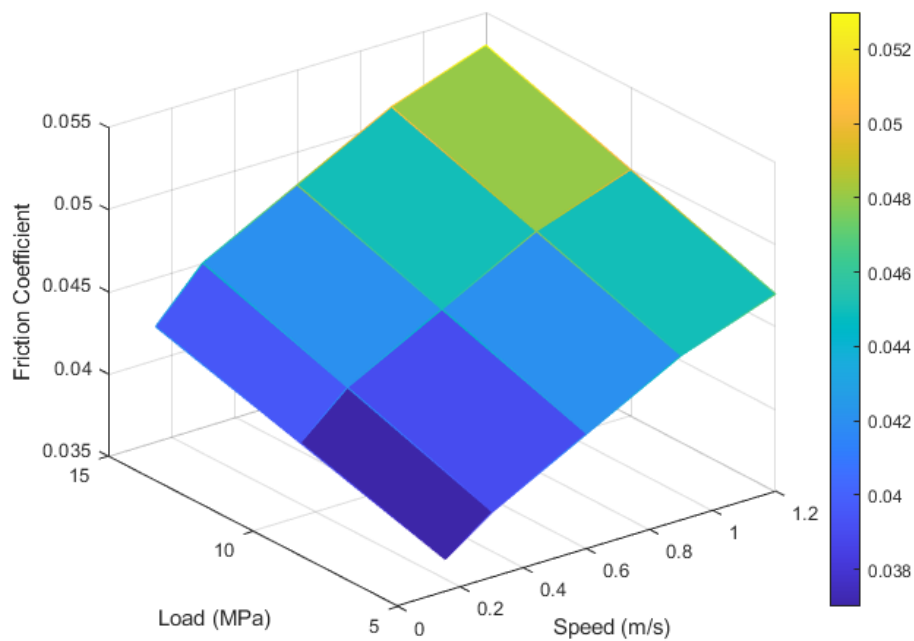
1. Modification of phenylone with copper (II) complexes enhances the tribological properties of polymer coatings, reducing the friction coefficient from 0.080 to 0.045 and improving wear resistance by 60%.
2. Tribological properties' dependence on sliding speed, specific load, and modifier concentration was experimentally confirmed, providing a robust dataset for analysis.

3. MATLAB processing yielded the analytical equation  $(V, P) = 0.0335 + 0.0095 \cdot V + 0.0005 \cdot P$  for coating No. 2, offering a reliable predictive tool for friction behavior.
4. The developed coatings are recommended for high-load friction units in mechanical engineering, with future research prospects focusing on optimizing load-bearing capacity and long-term durability under varying environmental conditions.



**Fig. 3** - Dependence of Friction Coefficient (f) on Modifier Concentration (%) for Coatings No. 2 and No. 3 at  $V = 0.6 \text{ m/s}$ ,  $P = 10 \text{ MPa}$

**Мал. 3** - Залежність коефіцієнта тертя (f) від концентрації модифікатора (%) для покриттів № 2 та № 3 при  $V = 0,6 \text{ м/с}$ ,  $P = 10 \text{ МПа}$



**Fig. 4** - Dependence of Friction Coefficient (f) of Coating No. 2 on Sliding Speed (V) and Specific Load (P)

**Мал. 4** - Залежність коефіцієнта тертя (f) покриття № 2 від швидкості ковзання (V) та питомого навантаження (P)

### Conflict of interest

The authors declare that there is no conflict of interest regarding the publication of the manuscript. In addition, the authors fully complied with ethical standards, including plagiarism, data falsification, and double publication.

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## МОДЕЛЮВАННЯ ТРИБОТЕХНІЧНИХ ВЛАСТИВОСТЕЙ ПОЛІМЕРНИХ ПОКРИТТІВ НА ОСНОВІ ФЕНІЛОНУ З МОДИФІКАТОРАМИ КОМПЛЕКСНИХ СПОЛУК МІДІ (II) ЗА ДОПОМОГОЮ MATLAB

**Мета.** Дослідження присвячено розробці та оцінці антифрикційних полімерних покриттів на основі фенілона C2, ароматичного поліаміду з високою термостійкістю, модифікованого комплексами міді (II) складу  $[\text{Cu}(\text{HL})\text{X}_2]_2$ , де HL – похідні ариламідів бензімідазол-2-тіокарбонової кислоти. Метою роботи є моделювання триботехнічної поведінки цих покриттів із акцентом на впливі швидкості ковзання, питомого навантаження та концентрації модифікатора для підвищення ефективності й довговічності вузлів тертя в машинобудівних вузлах за умов високих навантажень, характерних для промислового обладнання.

**Методи.** Покриття виготовляли шляхом розчинення фенілона C2 і модифікаторів комплексів міді (II) у диметилформаміді з подальшим просоченням пористої бронзової підкладки (пористість 20–25%) за вакуумного тиску протягом 30 хвилин. Зразки з покриттям піддавали термічному твердінню при 420 K протягом 1,5 години, а потім при 723 K протягом 2 годин для забезпечення повного затвердіння. Триботехнічні випробування проводили на машині тертя СМТ-2010 за схемою «колодка-диск» у змащеному середовищі з використанням індустріального масла І-40А (ГОСТ 20799-88). Дослідження охоплювали швидкості ковзання від 0,15 до 1,2 м/с і питомі навантаження від 5 до 15 МПа з контртілом зі сталі 45 (твердість 45–50 HV, шорсткість  $R_a$  0,4–0,63 мкм). Коефіцієнти тертя вимірювали з точністю  $\pm 0,001$ , а швидкість зношування визначали гравіметричним методом із точністю  $\pm 0,01$  мг/м після 10-годинних циклів випробувань. Експериментальні дані обробляли в MATLAB для виведення прогнозуючого рівняння коефіцієнта тертя.

**Результати.** Модифікація комплексами міді (II) значно покращила триботехнічні властивості покриттів на основі фенілона. При концентрації модифікатора 1% коефіцієнт тертя знизився з 0,080 до 0,045, а зносостійкість зросла на 60%. Покриття №2 (аніон Cl, замісник метоксифеніл) продемонструвало найкращі характеристики завдяки оптимальному поєднанню змащувальних властивостей і міцності. Обробка в MATLAB дала рівняння  $f(V,P)=0,0335+0,0095 \cdot V+0,0005 \cdot P$ , яке описує залежність коефіцієнта тертя від швидкості ковзання ( $V$ , м/с) і питомого навантаження ( $P$ , МПа) з максимальною похибкою менш ніж 5%. Оптична мікроскопія виявила утворення захисної трибохімічної плівки на поверхні контртіла, що зменшує знос завдяки зниженню прямого контакту та підвищенню гладкості поверхні.

**Висновки.** Розроблені покриття мають значний потенціал для використання у вузлах тертя з високими навантаженнями в машинобудуванні, забезпечуючи зниження тертя та підвищену зносостійкість у змащених умовах. Отримане рівняння є достатнім інструментом для прогнозування триботехнічної поведінки, що сприяє оптимізації конструкцій. Наявність трибохімічної плівки підкреслює важливість хімічних взаємодій у покращенні характеристик. Подальші дослідження можуть бути спрямовані на вивчення вищих концентрацій модифікатора (понад 1%) для оцінки меж деламінації та розширення застосовності покриттів до екстремальних температур і навантажень, характерних для сучасного промислового обладнання.

**КЛЮЧОВІ СЛОВА:** фенілон, комплекси міді, триботехнічні властивості, антифрикційні покриття, апроксимуючі рівняння.

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#### Конфлікт інтересів

Автори заявляють, що конфлікту інтересів щодо публікації рукопису немає. Крім того, автори повністю дотримувались етичних норм, включаючи плагіат, фальсифікацію даних та подвійну публікацію.

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