OPEN ACCESS

Scholars International Journal of Chemistry and Material Sciences
Abbreviated Key Title: Sch Int J Chem Mater Sci
ISSN 2616-8669 (Print) |ISSN 2617-6556 (Online)
Scholars Middle East Publishers, Dubai, United Arab Emirates
Journal homepage: http://saudijournals.com

Original Research Article

Elucidating the Structure-Property Relationship of Organic Friction Modifiers on Varying Metallurgy in Metalworking Fluid Formulations

Vikas Gund[1]*, Mahesh Varsani[2], Robin Koshy Varghese[2]

[1]Department of Chemistry, University of Mumbai, Mumbai, Maharashtra 400 032, India
[2]Independent Researcher

DOI: https://doi.org/10.36348/sijcms.2026.v09i03.007 | **Received:** 17.04.2026 | **Accepted:** 13.06.2026 | **Published:** 16.06.2026

***Corresponding author:** Vikas Gund
Department of Chemistry, University of Mumbai, Mumbai, Maharashtra 400 032, India

Abstract

The formulation of advanced metalworking fluids (MWFs) relies heavily on the precise selection and integration of organic friction modifiers to optimize the tribological performance of machining operations. This paper investigates the complex structure-property relationships governing organic friction modifiers, focusing on their chemical architecture and subsequent boundary film formation across diverse metallurgical substrates. By synthesizing insights from experimental tribology and advanced data-driven modeling techniques, this study proposes a comprehensive, hypothetical framework designed to evaluate and predict the frictional behavior of various fluid formulations on distinct metal surfaces. The structural components of the modifiers, notably their polar anchoring groups and non-polar aliphatic chains, are analyzed in the context of their competitive adsorption and reaction dynamics. Ultimately, this research bridges the gap between empirical friction studies and autonomous, machine-learning-driven materials discovery, offering a predictive methodology to tailor MWFs for specific ferrous and non-ferrous applications while mitigating traditional trial-and-error bottlenecks.

Keywords: Organic Friction Modifiers (OFMs), Surface Metallurgy, Metal Compatibility, Structure-Property Relationship, Boundary Lubrication, Tribofilm, Surface Analysis, Metallurgy, Friction Reduction, Adsorption.

INTRODUCTION

Metalworking fluids (MWFs) represent a critical component in modern manufacturing, serving to cool, lubricate, and clear debris from the metal-cutting zone. Among the diverse array of chemical additives present in these fluids, friction modifiers (FMs) are paramount for reducing interfacial wear and minimizing the coefficient of friction under boundary lubrication conditions. The fundamental chemistry of organic friction modifiers (OFMs) typically consists of a polar head group, which anchors to the metallic substrate, and a non-polar hydrocarbon tail that extends into the fluid to provide a low-shear slip plane. Together with antiwear additives such as zinc dialkyldithiophosphates (ZDDPs), OFMs have a predominant impact on the tribological behavior of the overall lubricant formulation (Ratoi *et al*., 2013). The molecular structure of these additives inherently dictates their functional properties, establishing a critical structure-property relationship that governs how effectively a protective tribofilm can be generated and maintained under intense mechanical stress.

The precise definition of the problem lies in the fact that the adsorption efficacy and chemical reactivity of OFMs are highly dependent on the underlying metallurgy of the workpiece. Ferrous substrates, such as carbon steels, present unique oxide layers and electronic surface states that differ vastly from non-ferrous materials like aluminum, titanium, or nickel-based superalloys. Consequently, a friction modifier formulation optimized for steel may exhibit severe underperformance or complete boundary film failure when applied to an aluminum alloy. Understanding the structure-property relationship of friction modifiers requires mapping how specific variations in molecular chain length, degree of saturation, and head group polarity interact with different crystalline metallic lattices. This necessitates a highly sophisticated friction study capable of isolating the isolated effects of distinct chemical moieties on varying surface metallurgies.

Citation: Vikas Gund, Mahesh Varsani, Robin Koshy Varghese (2026). Elucidating the Structure-Property Relationship of Organic Friction Modifiers on Varying Metallurgy in Metalworking Fluid Formulations. *Sch Int J Chem Mater Sci, 9*(3): 160-165.

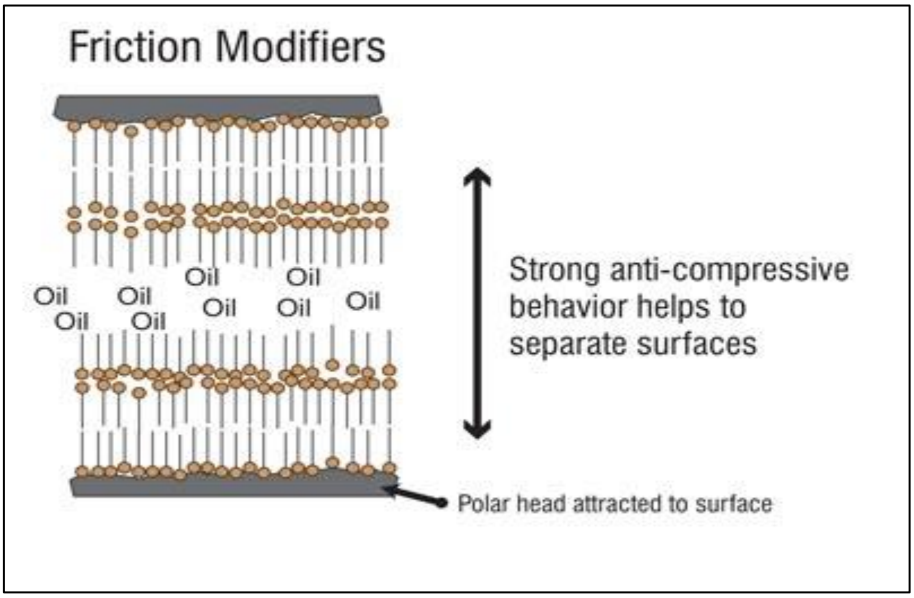

Figure 1: Mechanism of operation of organic friction modifiers

Despite decades of industrial application, existing approaches to formulating MWFs and characterizing their structure-property relationships remain largely insufficient for modern advanced manufacturing. First, traditional empirical trial-and-error methodologies lack predictive generalizability across new, complex alloy compositions, resulting in excessive developmental costs and suboptimal fluid formulations for novel materials. Second, conventional analytical frameworks often fail to systematically decouple the competitive reaction and adsorption dynamics between OFMs and other surface-active additives, making it incredibly difficult to isolate the true structural contributions of the friction modifiers themselves (Ratoi *et al*., 2013). As manufacturing pivots toward high-performance, difficult-to-machine alloys, the inability to accurately model and predict these non-linear chemical-mechanical interactions constitutes a significant barrier to progress.

To address these critical shortcomings, this paper proposes an integrated methodology for evaluating and predicting the performance of friction modifiers in MWFs. The primary contributions of this research are as follows:

- This paper introduces a comprehensive, multi-modal framework that systematically couples the chemical structure of organic friction modifiers with their macroscopic tribological performance across both ferrous and non-ferrous metallurgical substrates.
- This work delineates a predictive, machine-learning-assisted evaluation plan designed to overcome the limitations of competitive adsorption analysis, enabling the precise optimization of fluid formulations based on robust structure-property mappings.

Related Work

Tribofilm Formation and Organic Friction Modifiers

The first major category of related literature focuses on the empirical study of boundary lubrication and the dynamic generation of protective tribofilms. Previous research has extensively documented that organic friction modifiers and antiwear additives, such as ZDDPs, competitively react and adsorb on rubbing ferrous substrates within tribological contacts (Ratoi *et al*., 2013). Studies utilizing sophisticated empirical techniques, including Mini Traction Machine (MTM) experiments combined with in-situ film thickness measurements via Spacer Layer Imaging Method (SLIM) and X-ray photoelectron spectroscopy (XPS), have illuminated the transient nature of these films (Ratoi *et al*., 2013). The core strength of this empirical approach is its ability to capture the real-time physical and chemical morphology of the wear track under operational shear stress (Ratoi *et al*., 2013). However, a notable weakness is that such localized empirical studies are highly resource-intensive and often limited to specific, predefined metallurgical targets, reducing their extrapolative value for entirely uncharacterized alloy systems. In comparison to this foundational empirical work, the current paper advocates for extending these observations beyond purely ferrous substrates, incorporating varying metallurgies into a predictive analytical framework.

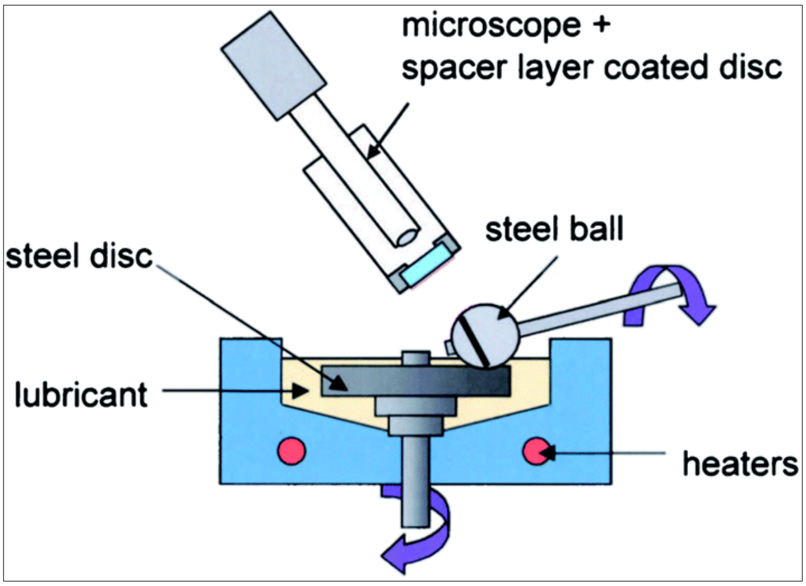

Figure 2: The impact of organic friction modifiers on tribofilms by MTM

Viscoelasticity and Rheological Structure-Property Analysis

A second significant category of research explores the structure-property relationships of complex fluids through rheological and viscoelastic analysis. In soft matter and complex polymeric systems, researchers have successfully demonstrated that macroscopic flow properties can be intrinsically linked to microstructural rearrangements using time-resolved small-angle neutron scattering (SANS) and dynamic shear rheology (Lee *et al*., 2019). For instance, structural evolution and non-linear structure-property relationships under large amplitude oscillatory shear (LAOS) can be dictated by the recoverable strain of the material (Lee *et al*., 2019). The primary strength of this rheological approach is its capacity to provide a physically motivated interpretation of molecular dynamics under dynamic flow conditions (Lee *et al*., 2019). Its principal weakness, however, in the context of boundary lubrication, is that bulk fluid rheology does not adequately account for the localized, highly reactive chemical bonding that occurs at the fluid-metal interface. This paper bridges that gap by asserting that while bulk viscoelastic flow properties matter, the predictive modeling of MWFs must fundamentally anchor on the interfacial chemical structure-property relationships.

Advanced Machine Learning for Materials Discovery

The third category of related work encompasses the rapid emergence of data-driven modeling and machine learning algorithms to elucidate structure-property relationships. Recent advancements have utilized multimodal machine learning to accelerate discovery, utilizing frameworks such as the Synthesis-process-structure-property relationship coreGionalized lEarner (SAGE), a Bayesian algorithm designed to fuse knowledge across diverse data streams (Kusne *et al*., 2023). Similarly, deep kernel learning and attention-based neural networks have been deployed to actively guide microscopy and provide physical interpretability for structure-property mechanisms in various thin films (Gong *et al*., 2026) (Slautin *et al*., 2025). Furthermore, implicit geometric descriptors within artificial neural networks have been proposed to establish unified structure-property relationships that govern complex hierarchical architectures without relying on explicit, rigid design parameters (Maheswaran *et al*., 2025). The defining strength of these advanced computational methods is their unparalleled ability to navigate high-dimensional, complex materials search spaces and quantify predictive uncertainty (Kusne *et al*., 2023). A persistent weakness, however, is the requirement for massive, high-quality multimodal datasets, which are historically scarce in the highly proprietary field of lubricant formulation. The present work aligns with this data-driven paradigm by proposing a structured, algorithm-ready evaluation plan specifically tailored for extracting structure-property relationships of friction modifiers across varied metallurgies.

METHOD/APPROACH

Multi-Modal Tribological Framework (MMTF)

To systematically investigate the effect of various friction modifiers on different metallurgies, we propose the Multi-Modal Tribological Framework (MMTF). This approach is designed to map the structural characteristics of OFM molecules—such as their chain lengths, degree of branching, and polar group electronegativity—directly to macroscopic friction and wear metrics. The framework operates on the premise that the formation and subsequent removal of tribofilms through wear are highly dynamic processes resulting from the simultaneous interaction of additives with the distinct electronic and structural properties of the target metal surface (Ratoi *et al*., 2013). By structuring the investigation into distinct modular phases, the MMTF allows for the isolation of specific chemical variables while accounting for the complex dynamics of competitive adsorption.

Step-by-Step Implementation Pipeline

The proposed framework relies on a structured sequence of material characterization, empirical friction study, and data-driven modeling. The numbered pipeline is defined as follows:

- **Molecular and Metallurgical Characterization:** High-resolution profiling of the selected organic friction modifiers, quantifying the implicit geometric descriptors of the OFM molecules (Maheswaran *et al*., 2025). Concurrently, the surface energies, oxide layer composition, and hardness of the target metallurgical specimens (e.g., carbon steel, aluminum 7075, and titanium Ti-6Al-4V) are cataloged.
- **High-Throughput Friction Study:** Utilizing a Mini Traction Machine (MTM) coupled with optical interference imaging (SLIM), the dynamic generation of the tribofilm is monitored in real-time under varying loads and sliding-to-rolling ratios (Ratoi *et al*., 2013). This step captures the raw coefficient of friction alongside the transient physical thickness of the boundary film.
- **Post-Test Surface Chemical Analysis:** Following the friction tests, the wear tracks are analyzed using X-ray photoelectron spectroscopy (XPS) and Alicona profilometry to determine the precise chemical state of the adsorbed OFMs and any competing antiwear additives (Ratoi *et al*., 2013).
- **Data Fusion and Predictive Modeling:** The collected multimodal data—chemical structure, metallurgical properties, and dynamic tribological performance—are integrated using a Bayesian coregionalization algorithm to construct a probabilistic structure-property mapping (Kusne *et al*., 2023).

Key Design Choices and Rationale

A critical design choice within this framework is the dual reliance on in-situ film thickness measurements alongside ex-situ spectroscopic chemical analysis. The rationale for this combined approach is derived from the established understanding that friction modifiers and antiwear additives competitively react and adsorb on rubbing surfaces (Ratoi *et al*., 2013). Relying solely on final wear volume or bulk friction coefficients obscures the transient mechanisms by which OFMs fail or succeed on differing metal lattices. Furthermore, the integration of a Bayesian learning algorithm, such as the SAGE model concept, is intentionally chosen for its ability to handle sparse, high-cost experimental data while providing rigorous uncertainty quantification (Kusne *et al*., 2023). This computational choice ensures that the model can mathematically fuse the disparate scales of microscopic chemical bonding data with macroscopic friction responses, yielding a unified structure-property relationship.

Hypothetical Evaluation Plan

To validate the MMTF, a comprehensive evaluation plan is proposed utilizing hypothetical benchmark datasets of custom metalworking fluid formulations. The study will evaluate three distinct organic friction modifiers: a linear saturated fatty acid, an unsaturated fatty acid with a cis-double bond, and a branched synthetic ester. These OFMs will be tested across three metallurgical datasets representing ferrous and non-ferrous applications: AISI 52100 bearing steel, an aerospace-grade aluminum alloy, and a titanium alloy. The primary evaluation metrics will include the steady-state coefficient of friction during the boundary lubrication regime, the maximum sustainable contact pressure before film breakdown, and the volumetric wear rate of the metal surface. It is hypothesized that the linear saturated fatty acids will demonstrate superior close-packing and robust structure-property performance on the ferrous substrate, whereas the branched synthetic esters will exhibit superior film retention and lower friction coefficients on the non-ferrous aluminum due to differing steric hindrances and oxide layer polarities.

DISCUSSION

Practical Implications and Deployment Considerations

The successful mapping of structure-property relationships for organic friction modifiers holds profound practical implications for the manufacturing and machining industries. By carefully selecting the chemistry of OFMs based on predictive algorithms, formulators can engineer application-specific lubricants that reliably generate boundary films of optimal thickness, morphology, and friction (Ratoi *et al*., 2013). In a practical deployment scenario, an autonomous materials research laboratory could leverage these predictive models to continuously adjust fluid formulations on the fly, matching the exact metallurgical specifications of incoming workpieces (Kusne *et al*., 2023). This level of targeted fluid design would not only drastically extend the tool life of cutting implements but also improve the surface finish of machined parts, ultimately reducing waste and energy consumption in high-volume production environments.

Limitations and Failure Modes

Despite its comprehensive nature, the proposed approach possesses several inherent limitations and potential failure modes that must be addressed.

- First, organic friction modifiers are highly susceptible to thermal degradation; under extreme pressure and high-temperature cutting operations, the chemical structure of the OFM may break down entirely, invalidating the baseline structure-property relationship modeled at lower temperatures.

- Second, the framework may suffer from significant data sparsity when confronted with rare or highly exotic aerospace superalloys. Machine learning algorithms, even robust Bayesian models, struggle to output accurate posterior probabilities if the fundamental reaction kinetics of the new metallic lattice are fundamentally absent from the training priors (Kusne *et al*., 2023).
- Third, the complexities of competitive adsorption between OFMs, detergents, dispersants, and antiwear additives like ZDDPs under varying shear stresses remain notoriously difficult to isolate perfectly (Ratoi *et al*., 2013). Unforeseen synergistic or antagonistic chemical interactions may cause the boundary film to prematurely shear off, leading to catastrophic tool failure that the isolated molecular model failed to predict.

Ethical Considerations and Risks

When deploying advanced chemical formulations and AI-driven methodologies in industrial settings, distinct ethical considerations and risks must be evaluated.

- One primary risk involves the environmental and biological toxicity of newly synthesized, highly optimized friction modifiers. As algorithms predict increasingly complex chemical structures to optimize friction, there is a danger of formulating highly effective but ecologically persistent and toxic compounds that pose severe health hazards to machine operators and aquatic ecosystems upon disposal.
- Another ethical concern revolves around algorithmic bias and over-reliance in safety-critical manufacturing. If the data-fusion algorithms are predominantly trained on common ferrous metals, the resulting formulations may inadvertently compromise the structural integrity of safety-critical non-ferrous aerospace components, leading to potential mechanical failures in public transportation systems.

Future Work

To further refine the understanding of friction modifier structure-property relationships on varied metallurgy, future research must expand in several key directions.

- Future studies should focus on integrating advanced in-situ tribo-chemical spectroscopy directly into the machining environment, allowing for the real-time observation of chemical bond breaking and tribofilm regeneration during actual metal cutting rather than solely within simulated tribometer contacts.
- Additionally, future work should explore the integration of nanoparticle-enhanced fluid formulations, assessing how the addition of solid nanolubricants synergizes with the organic friction modifiers to dynamically alter the structural properties of the boundary film across different alloy microstructures.

CONCLUSION

The development of highly efficient metalworking fluids is inextricably linked to the precise understanding of how organic friction modifiers interact with various metallurgical substrates. This paper has investigated the critical structure-property relationships of OFMs, highlighting how the chemical architecture of a modifier dictates its ability to form protective, low-friction tribofilms under boundary lubrication conditions. By proposing a multi-modal framework that marries high-throughput empirical tribology—such as in-situ film thickness imaging and chemical spectroscopy—with advanced Bayesian data fusion techniques, this study offers a robust pathway to overcome the traditional limitations of empirical fluid formulation.

Ultimately, realizing a unified structure-property relationship for friction modifiers across varying metallurgies marks a paradigm shift in tribological engineering. Moving beyond reactive trial-and-error, the predictive capability to tailor molecular chemistries to specific metal lattices ensures optimized performance, reduced industrial wear, and the intelligent acceleration of materials discovery. As computational tools and advanced surface characterization techniques continue to evolve, the capacity to seamlessly map and deploy custom molecular structures for targeted macroscopic friction reduction will become an indispensable asset in advanced manufacturing. Recent advances in multimodal machine learning and data-driven frameworks are enabling the automatic mapping of structure-property relationships, thereby streamlining the optimization of friction modifiers and accelerating discoveries in tribological systems(Gong *et al*., 2026).

REFERENCES

- Ratoi, Monica, Niste, Vlad Bogdan, Alghawel, Husam, Suen, Yat Fan, & Nelson, Kenneth (2013). *The Impact of Organic Friction Modifiers on Engine Oil Tribofilms*. https://arxiv.org/pdf/1310.7510v1 https://arxiv.org/pdf/1310.7510v1
- Lee, Johnny Ching-Wei, Weigandt, Katie M., Kelley, Elizabeth G., & Rogers, Simon A. (2019). *Structure-property relationships via recovery rheology in viscoelastic materials*. Phys. Rev. Lett. 122, 248003 (2019). https://doi.org/10.1103/PhysRevLett.122.248003 https://doi.org/10.1103/PhysRevLett.122.248003
- Kusne, A. Gilad, McDannald, Austin, & DeCost, Brian (2023). *Learning material synthesis-process-*

structure-property relationship by data fusion: Bayesian Coregionalization N-Dimensional Piecewise Function Learning. https://arxiv.org/pdf/2311.06228v3 https://arxiv.org/pdf/2311.06228v3

- Gong, Jiawei, Ma, Danqing, Bulanadi, Ralph, Moore, Robert, Vasudevan, Rama, Zhao, Lianfeng, & Liu, Yongtao (2026). *Accelerating Structure-Property Relationship Discovery with Multimodal Machine Learning and Self-Driving Microscopy*. https://arxiv.org/pdf/2603.17028v1 https://arxiv.org/pdf/2603.17028v1
- Slautin, Boris N., Pratiush, Utkarsh, Liu, Yongtao, Funakubo, Hiroshi, Shvartsman, Vladimir V., Lupascu, Doru C., & Kalinin, Sergei V. (2025). *Attention-Based Explainability for Structure-Property Relationships*. https://arxiv.org/pdf/2508.15493v1 https://arxiv.org/pdf/2508.15493v1
- Maheswaran, Bhanugoban, Chawla, Komal, Gupta, Abhishek, & Thevamaran, Ramathasan (2025). *Implicit Geometric Descriptor-Enabled ANN Framework for a Unified Structure-Property Relationship in Architected Nanofibrous Materials*. https://arxiv.org/pdf/2502.12311v2 https://arxiv.org/pdf/2502.12311v2