FROM ELBOW GREASE TO ARTIFICIAL INTELLIGENCE: OPTIMIZING GREASE FORMULATIONS

The formulation of industrial lubricants, particularly grease, has traditionally been an arduous process that requires hundreds of manual tests and significant financial investment. As global industries strive to reduce the 20–23% of energy currently lost to friction and wear, artificial intelligence (AI) and machine learning (ML) have emerged as transformative tools to accelerate lubricant research and development. This paper explores the transition from traditional trial-and-error methods to data-driven approaches, highlighting the efficacy of supervised learning and deep learning (DL) models, such as artificial neural networks (ANNs), in predicting the coefficient of friction (COF) and wear scar diameter (WSD). Despite its potential to reduce lubricant development time by up to 70% and overall costs, the integration of AI faces significant hurdles, including data scarcity, model complexity, and limited transferability across operating environments. This study reviews current ML applications, addresses the socio-technical challenges of implementation, and evaluates emerging solutions such as physics-informed machine learning (PIML) and the development of standardized, shared databases. Ultimately, the synergy between AI and tribology offers a pathway toward reducing energy loss in industry, as well as formulating more sustainable bio-based lubricants.

Introduction:

The importance of lubricants is often overlooked, as they are a less glamorous application of engineering. Nonetheless, lubricants are essential to the functioning of nearly every industry on Earth, especially those that rely on heavy machinery and engines, such as automotive, manufacturing, mining, and construction. Lubricants reduce friction and wear, therefore preserving machinery and reducing energy costs. Currently, 20–23% of global energy is lost on friction and wear, and 30–40% of machine failures result from these issues over time [1]. Current lubricant technology is used in a myriad of industries but suffers from flawed formulations due to the intense and complex environments that labs struggle to recreate under time and cost constraints. The result of these barriers is that wear is not always limited to the extent desired, resulting in continued energy loss and mechanism failure over time.

Developing new formulations for lubricants that will better suit individual industries is incredibly time-consuming. Normally, creating lubricants takes 50–200 tests and months of work. An emerging tool that can help reduce this research and development time is AI. It can improve the formulation of lubricants by reducing the effort of production, such as the number of tests and the time, by 40–70% if provided with a quality dataset and formulation spaces, while maintaining 90–97% accuracy while predicting lubricant features such as friction coefficients, wear rates, and lubricant film thickness. AI can also improve production efficiency by 15–30% [1]. Current research in machine learning is working to decide the best models for application in lubricant formulation.

Grease as a lubricant and its formulation:

Lubricant is an umbrella term that encapsulates oils, greases, solids, and penetrating agents that reduce friction and wear. Grease is an oil-based product that can form in solid to semi-fluid forms, and is designed to stay in place, seal, and protect. Traditionally, developing a new grease involves mixing various base oils, thickeners, and additives in different ratios and testing them manually, which is both time-consuming and expensive.

Its general formula is shown in the equation below :

Grease = Base Oil + Thickener + Additives
(1)

80-90% 5-15% 2-7%

The base oils used in grease are either mineral or synthetic. Grease is typically classified into two categories: soap-based and non-soap-based, depending on the thickeners used in its formulation. Soap-based grease uses a soap, such as lithium or calcium 12-hydroxy stearate, to form a network that holds the base oil in place and gives the grease its semi-solid consistency, allowing adhesion at frictional interfaces. Soap-based grease is commonly used in various industrial applications due to its good water resistance and ability to lubricate at low temperatures. On the other hand, synthetic grease, or non-soap-based grease, employs a synthetic thickener, such as polyurea, to give the lubricant its structure and offers better lubrication, wear prevention, and high-temperature stability, as well as higher resistance to water washout [2]. Fig. 1 shows a flowchart of common types of greases, including several mentioned above. These classifications prove important as they define the grease's foundational structure, meaning an AI model must treat them as separate chemical spaces with unique processing rules, compatibility constraints, and performance limits.

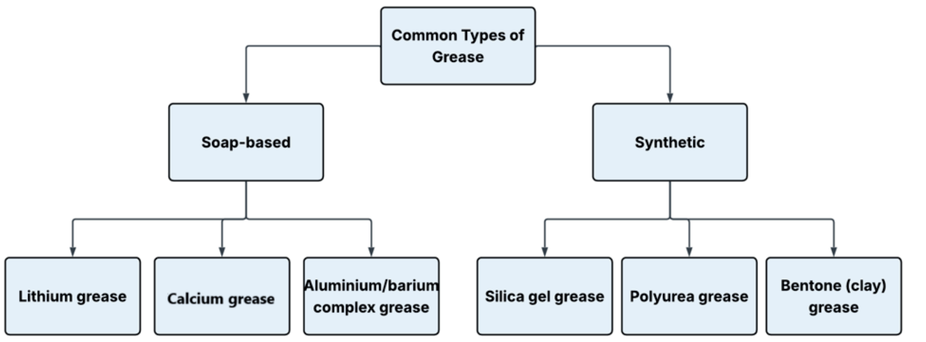

Fig. 1. Common Types of Greases. Adapted from [2].

A myriad of different additives are used to enhance performance and protect grease. The most common additives are antioxidants, corrosion inhibitors, extreme pressure, anti-wear, viscosity index improvers, and friction modifiers [3].

Additives are an imperative part of formulating high-performance greases, but it is difficult to manually optimize them. The dispersibility of additives, such as nanoparticles, is fundamental to successful implementation, but many additives can clump together or fail to mix smoothly into base materials. Additives may exhibit synergistic or antagonistic interactions, and these effects are often highly nonlinear. A solution to this dilemma is chemical functionalization, where an additive's surface or molecular structure is chemically altered to add new functionalities [4]. Additives already have highly competitive, non-linear relationships, and chemical functionalization increases the complexity of the relationships. Due to the sensitivity of a grease to additive changes, predicting the outcome of an adjustment or addition mathematically without specialized software or large amounts of trial-and-error testing is arduous. The challenge with grease formulation is testing for the different properties of base oils, thickeners, and additives when they are combined in different environments and ratios. Also, grease is fundamentally a rheological material, and other parameters like the following will heavily influence its performance: Yield stress, viscoelasticity, storage modulus (G'), and loss modulus (G").

Tribology is the science and engineering of interacting surfaces in relative motion, encompassing the study of friction, wear, and lubrication, and therefore relevant to grease formulation [5-6]. There are millions of possibilities and variations, each with different applications in individual industries, which is where AI in machine learning and deep learning can help to improve formulation efficiency.

Foundation of machine learning models in formulation:

Machine learning (ML) is a subset of AI that involves training algorithms to make predictions or decisions based on given data. These algorithms learn from past experiences or patterns in data so they can perform tasks without being explicitly programmed to do so, but their reliability and generality are impacted by the size of the data sets used to train the models. Larger data sets result in more diverse and representative samples, and size influences computational requirements, training time, and the complexity of the chosen model [7].

AI can improve lubrication formulation using ML and Deep Learning (DL) models to predict performance by analyzing large datasets of grease properties, such as viscosity, thermal stability, and flash point, to predict how a new mixture will behave before it is made in a lab. These models can also optimize complex recipes. Grease behavior is non-linear, meaning small changes in one additive can have huge effects on wear, and AI identifies hidden patterns that could be otherwise missed [8]. Having said this, actual grease properties depend heavily on saponification conditions, reaction temperature, cooling rate, milling/shearing, dehydration conditions, and worker process variability. Two identical formulations can yield different grease performance. There are some variables which often are as important as grease chemistry, such as worked penetration, mechanical stability, dropping point, bleed, oxidation stability, and roll stability.

Scientists have explored many fundamental algorithms for lubrication, and a few of them have repeatedly appeared in tribological studies, such as logistic regression, support vector machines, discriminant analysis, Bayesian modeling, decision trees, and artificial neural networks (ANN) [8]. These models can predict key parameters for lubricants. Table 1 shows the different ML approaches and what predictive applications they are best suited for. The table exemplifies how ANNs are by far the most versatile approach in tribological data predictions.

Machine learning approach	Predictive applications and uses
Artificial Neural Networks (ANNs)	*Operating conditions related to friction and wear *Performance parameters (COF, WSD) • Lubrication film thickness & identifying the lubrication regime • Friction and wear for a given experimental condition
Discriminant Analysis	• General experimental parameters
Bayesian Modeling	• General experimental parameters
Transfer Learning	• General experimental parameters
Logistic Regression	• Lubrication film thickness • Identifying the lubrication regime
Support Vector Machine (SVM)	• Friction and wear for a given experimental condition
Polynomial Regression	• Friction and wear for a given experimental condition

Table 1. ML approaches and their predictive applications. Adapted from [8]

In this paper, we focus on COF and WSD, but we do not ignore the importance of other critical grease properties including but not limited to: NLGI grade, dropping point, oil separation, water washout, water spray-off, corrosion resistance, low-temperature torque, oxidation life, and bearing life.

In an experiment testing the accuracy of a selection of ML models for use in biodiesel production, Azhar et al. show the R2 mean values for various ML models across different values of K in Fig. 2, where K represents different configurations or folds in cross-validation [7]. Although the data is not specific to grease formulation, it is transferable because ML model analysis for biodiesel production translates well to grease formulation optimization since both rely on predicting nonlinear responses based on varying input parameters. The R^2 mean value measures the accuracy of the model's predictions, with values closer to one indicating better performance. Most of the high-performing models in this figure are supervised learning models based on decision trees, exemplifying how these models can take data sets and accurately predict outcomes based on current knowledge.

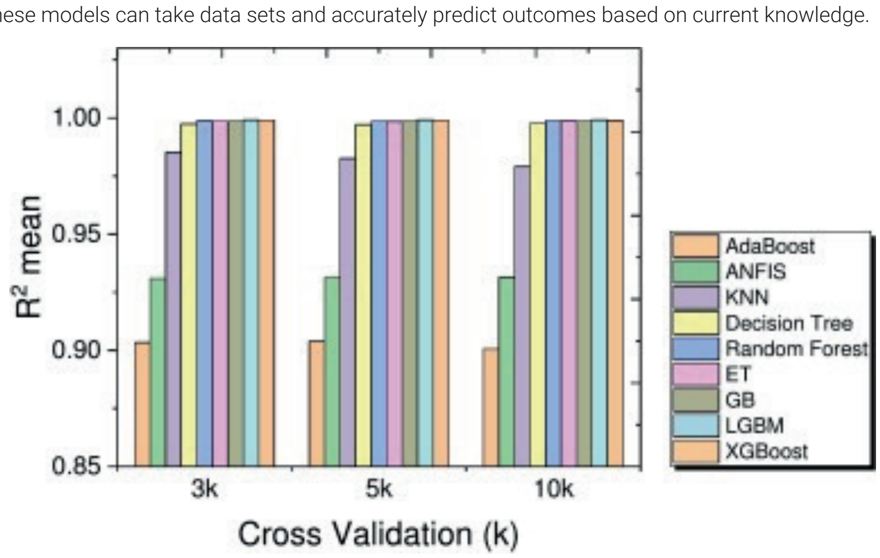

Fig. 2. Machine learning model analysis [7].

Deep learning models differ from machine learning models because they use multi-layered artificial neural networks to automatically learn patterns from large, unstructured data with minimal human intervention. Fig. 3 shows the neural network architecture for predicting COF and WSD in lubricated four-ball tribo-tests [9]. The network is a multilayer perceptron (MLP) neural network, which is a type of ANN composed of an input layer, one or more hidden layers, and an output layer. As seen in the figure, the inputs consist of lubricant properties, separate additive properties, and operating conditions. The layers consist of neurons that are each connected to every neuron in the subsequent layer. A connection carries weights that are iteratively updated during training to minimize prediction error, and non-linear activation functions are applied between layers so the network can capture intricate patterns and non-linear relationships that are part of a tribological dataset. The experiment the trained neural network shown in Fig. 3 was utilized in, performed by Granja and Higgs, demonstrated a strong and consistent predictive performance. For the COF, the model achieved an R2 of 0.8425, and for the WSD, an R2 of 0.9903 on the testing set [9]. The WSD likely had a more accurate prediction because it is a measurement of the physical damage left on a surface, and therefore a cumulative macroscopic metric, whereas COF is a highly dynamic microscopic property that is affected by highly unpredictable surface phenomena.

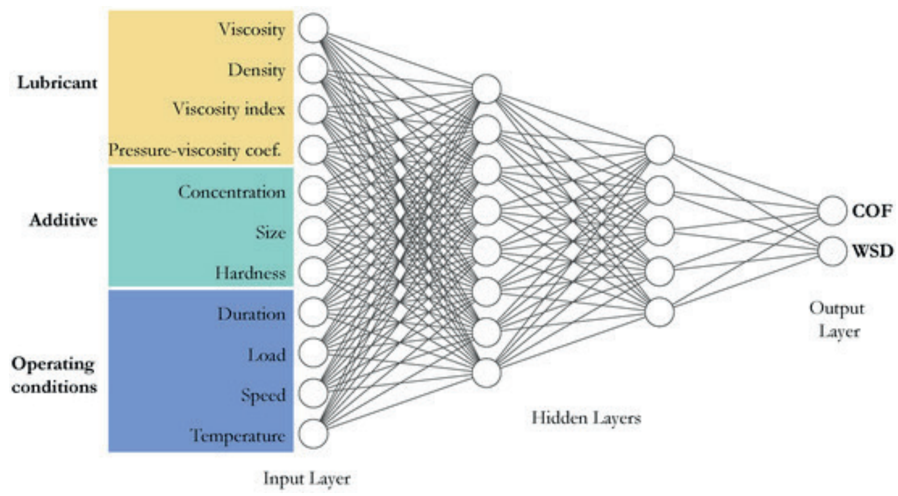

Fig. 3. Multilayer perceptron (MLP) neural network [9].

Challenges with ML and DL models in the grease industry:

Challenges presented by ML and DL models include limited data, complex interactions, hard-to-understand models, and privacy issues. Table 2 summarizes these issues and presents possible improvements that can be implemented in the future as AI use in the lubrication industry grows.

Table 2. Summary of key challenges with ML and DL models in application for lubricants [1, 10, 11].

Challenge	Description	Possible improvements
Scarcity of quality data	Tribological systems entail mechanical interactions, thermal interactions, chemical interactions and material interactions that happen at different sizes, making uniform quality data difficult to obtain and organize. To be exact, subjects like but not limited to: • additive compatibility • thickener compatibility • manufacturing process constraints • cost constraints • supply-chain constraints • OEM approvals • environmental regulations We know that a model that predicts low wear is useless if: • additive package is incompatible, • grease fails mechanical stability, • grease cannot be manufactured.	Development of shared databases, and adoption of standardized datasets streamlined by automated data acquisition pipelines.
Complex environment-dependent interactions	Predictions often fail when applied to different operating environments or grease formulations.	Integration of physics-informed and hybrid models.
Usability and trust	Models are often difficult to understand and provide limited transparency, resulting in distrust among the engineers and technicians using them.	Implement explainable AI models, user-friendly dashboards, ethical safeguards, and frameworks with human interaction that include expert validation with data-driven predictions.
Privacy issues	Data from sensors, maintenance records, and production systems is not available to researchers because of privacy and intellectual property rules.	Creation of industry-wide encrypted edge architecture cloud layers that enable protected joint learning and model training.

The scarcity of quality data sets is the most serious challenge to the application of AI in lubricant formulation optimization, as tribological systems are highly complicated. They must account for mechanical interactions, heat interactions, chemical interactions, and material interactions, all occurring at different sizes, from tiny atomic contacts of around 10 nm to large sliding surfaces. In many industries, more than 70–80% of the data from sensors, maintenance records, and production systems is not available to researchers because of privacy and intellectual property rules, and only 20–30% of industrial datasets are publicly available, which limits the development and testing of robust ML models [1]. Developing shared databases with standardized data sets would improve the industry, but every company would have to be willing to participate to also reap the benefits. If an agreement on sharing data cannot be made, the widespread application of AI in lubricants will take far longer and may even be impossible at an efficient output level.

Shared databases would have to be accomplished carefully with consideration for privacy regulations and cybersecurity. Large data centers are at risk for both theft and manipulation. Secure cloud–edge–end collaboration can mitigate these threats while still enabling data to be shared between different entities [12].

Trust in AI also proves to be an issue. Many models make it difficult to track where the information is produced from, so engineers and technicians are wary of their results. To guarantee the validity of the responses through expert confirmation, explainable AI models can be implemented. Explainable models are ML systems designed to be understood, interpreted, and trusted by humans, so ideally, they will build more trust with their intended users. In a meta-analysis on the correlation of trust and explainability in AI, Zahra Atf and Peter Lewis found a correlation coefficient of 0.194, which indicates a statistically significant but low positive correlation between the explainability of artificial intelligence and trust [13]. Their findings suggest that while explainability does indeed bolster trust, it does not wholly solve the dilemma of trust in AI. The addition of complementary factors such as user-friendly dashboards, ethical safeguards, and frameworks that incorporate expert validation can further build user trust.

AI predictions often fail when they are removed from the lab environments in which they were tested and applied in operating environments or with new grease formulations. For better AI grease formulation, it is critical to consider and include the following: molecular descriptors, Hansen solubility parameters, viscosity, elemental composition, additive concentration, and thickener type. The next generation of physics-informed ML models could be the solution and will be discussed further below.

Artificial Intelligence sustainability:

Energy use is often a concern with the use of AI. Although ML and DL models use large amounts of energy in their training stages, they are very efficient in the application phase relative to running experiments and simulations. The energy reaches a break-even point, where the time/energy saved by not running full simulations covers the cost of training. For example, in a study by S. Cartwright et al., it was determined that the expected break-even point for energy expenditure was reached after evaluating the neural network models around 8900 times [14].

Although AI can make up for its energy consumption, there are significant concerns with its emissions and water use. Considering that the ANNs are slightly different from typical lubricant formulation models, training AI models such as ANNs can emit more than 626,000 pounds of carbon dioxide equivalent [15]. In an age where many industries are trying to cut their emissions to combat climate change, the large emissions of AI are a serious hindrance. AI models also consume significant amounts of water. Currently, there are no systematic studies on the AI industry and its water consumption, but initial research shows that AI has a significant water footprint because it uses water both for cooling the servers that power its computations and for producing the energy it consumes [16]. The excessive use of water by AI models will become a larger issue as algorithms are increasingly used in a variety of industries and in everyday life. Applying AI to lubricant formulation will only worsen the dilemma of water consumption and carbon dioxide emissions unless solutions to the above issues are found.

While the use of AI can harm the environment, it also has the potential to transform business practices and industries and address major societal problems, including sustainability. AI has unique capabilities in data analysis and can integrate thousands of computers and other resources to solve complex problems. It can therefore be leveraged to find ways to mitigate the climate crisis if used correctly [17]. In grease formulation, it can mitigate energy wasted on the manual formulation process, as well as help determine the lowest energy methods for lubrication formulation and what materials are most sustainable for a desired grease. Companies utilizing AI should make the decision to include sustainability goals in their AI use, so they can achieve optimization as well as improved sustainability.

Future of machine learning in lubricants:

AI shows potential for extreme growth, especially in grease formulation optimization. As of right now, ML models do not account for sustainability considerations, but with improvements to their data systems, they can not only work with environmental considerations but also be the stepping-stone to help industries meet environmental standards without sacrificing mechanical reliability. Conventional lubricants contain chemical additives that are harmful to health and the environment. AI can be leveraged to assess the feasibility of replacing conventional lubricants with bio-based lubricants. Soares et al. found that multiple bio-based greases met vibration pattern similarity to conventional commercial grease (white - Calcium 8 - 10%) of 95% or higher using AI [18]. Their results prove that bio-based lubricants have the potential to meet industry standards and that AI can aid in formulation and testing methods to reach industry goals.

For AI in the lubricant industry to be able to grow, large databases must be put into place. Future research should aim to create open databases containing experimental findings, simulation data, and industrial records, with the safety precautions mentioned in the challenges section of this paper. These databases could include details like friction coefficients ($\mu \approx 0.01$–1.0), wear rates (10^{-9}–10^{-3} mm^3 /N·m), and surface roughness (Ra ≈ 0.02–5 μm). The addition of information from laboratories worldwide could increase the size of common databases by 520 times, resulting in better support for AI models in tribology everywhere [1].

Lastly, new opportunities will emerge through physics–AI models. These models integrate physics-based knowledge into machine learning models. Physics-informed machine learning (PIML) is a new tool for understanding and optimizing phenomena related to friction, wear, and lubrication. Traditional machine learning approaches often lack the incorporation of fundamental physics, as they rely solely on data-driven techniques of analysis. An example is the Archard wear law, which is a simple model used to describe sliding wear and is based on the theory of asperity contact. Archard's wear equation can lack complete generality, but when paired with machine learning causal depth and flexibility is introduced to wear modeling in a manner that the Archard model lacks [19]. PIML approaches, such as Physics-Informed Neural Networks (PINNs), leverage the known physical laws and equations to guide the learning process, leading to more accurate, interpretable, and transferable models [20]. These models have the potential to solve the problem of non-transferable predictions in current ML models.

Conclusion:

The integration of AI in lubricant and grease formulation marks a pivotal shift in tribology, moving from a labor-intensive discipline that requires months of work and high testing needs to a predictive science. By leveraging machine learning and deep learning models such as ANNs and Decision Trees, researchers can navigate the non-linear complexities of chemical additives and base oil interactions with unprecedented speed and accuracy.

However, challenges such as universal data access, transferability of predictions, privacy, and trust in AI remain as primary obstacles in widespread adoption. To achieve the full potential of these digital tools, the industry must move toward a collaborative system consisting of encrypted, shared databases and explainable AI frameworks that benefit all parties in the industry.

Further opportunities for growth and improvement in AI for application in grease formulation is seen in the evolution of Physics-Informed Machine Learning, which shows promise to bridge the gap between pure data-driven predictions and the fundamental laws of mechanics, ensuring that models remain robust outside of controlled laboratory settings. Furthermore, AI can serve as an enabler for the green transition, providing the computational power necessary to optimize bio-based alternatives that can match the reliability of traditional lubricants with fewer dangerous chemicals and from more sustainable sources. As these technologies mature, AI combined with tribology has the potential to reduce global energy waste and redefine the boundaries of material science and industrial sustainability.

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Biographies

Dr. Raj Shah, is a Director at Koehler Instrument Company in New York, where he has worked for the last 25+ years. He is an elected Fellow by his peers at ASTM, IChemE, ASTM, AOCS, CMI, STLE, AIC, NLGI, INSTMC, Institute of Physics, The Energy Institute and The Royal Society of Chemistry. An ASTM Eagle award recipient, Dr. Shah recently coedited the bestseller, “Fuels and Lubricants handbook”, details of which are available at ASTM’s Long-awaited Fuels and Lubricants Handbook https://bit.ly/3u2e6GY. He earned his doctorate in Chemical Engineering from The Pennsylvania State University and is a Fellow from The Chartered Management Institute, London. Dr. Shah is also a Chartered Scientist with the Science Council, a Chartered Petroleum Engineer with the Energy Institute and a Chartered Engineer with the Engineering council, UK. Dr. Shah was recently granted the honorific of “Eminent engineer” with Tau beta Pi, the largest engineering society in the USA. He is on the Advisory board of directors at Farmingdale university (Mechanical Technology), Auburn Univ (Tribology), SUNY, Farmingdale, (Engineering Management) and State university of NY, Stony Brook (Chemical engineering/ Material Science and engineering). An Adjunct Professor at the State University of New York, Stony Brook, in the Department of Material Science and Chemical Engineering, Raj also has over 700 publications and has been active in the energy industry for over 3 decades.

Ms. Anjali Batra is part of a thriving internship program at Koehler Instrument Company in Holtsville, NY underneath Dr. Raj Shah. Batra is also a student in the department of Chemical Engineering at Tufts University with a minor in engineering management.


Anjali Batra


Kate Marussich

Ms. Kate Marussich is part of a thriving internship program at Koehler Instrument Company in Holtsville, NY underneath Dr. Raj Shah. Marussich is also a student in the department of Material Science and Chemical Engineering at Stony Brook University, where Dr. Shah serves on the External Advisory Board.


Carl Kemizan

Dr. Carl F Kernizan Received his BS in Chemistry in 1982 from City College of NY (CCNY), his Ph.D. in Physical Chemistry in 1987 from City University of NY (CUNY) and Post-Doctoral degree from Kansas State University (KSU) in 1989. He worked in various technical and commercial roles from 1990 to 2017 as Principal Research Chemist with the Timken Company, Industrial Product Manager in Europe, North and Latin America with the Lubrizol Corporation, Technical Director with Jesco Resources Inc, VP of Business Development & Corporate Strategy with Axel Americas LLC and Chief Corporate Chemist with Warren Oil. He founded KV Tech Consulting LLC with his wife Sheila in 2017. He has consulted for multiple additive and grease companies and was hired to build R&D laboratories, oil blending and grease plants in the industry. He has authored over thirty articles in nanomaterials, spectroscopy, Newtonian fluids, grease formulations and tribology. He also owns a patent in “Metal Hydroxide Desiccated Emulsions used to Prepare Grease” PCT/US03/25447 and another in “Colloidal Suspension for Use as a Lubricant or Additive” Serial No: 08/175,312.


Behshad Sabah

Behshad Sabah, P.Eng. is a Mechanical Engineer and Senior Technical Advisor with over 29 years of international experience in lubrication engineering, tribology, reliability, condition monitoring, and industrial maintenance across the oil & gas, mining, steel, manufacturing, energy, and heavy industrial sectors. He holds a Bachelor’s degree in Mechanical Engineering and is a licensed Professional Engineer (P.Eng.) in Ontario. His credentials include STLE Certified Lubrication Specialist (CLS), NLGI Certified Lubricating Grease Specialist (CLGS), Oil Monitoring Analyst (OMA/OMX), and Vibration Analyst Categories I and II. Currently with Petro-Canada Lubricants (HF Sinclair), he provides technical leadership in equipment reliability, lubrication optimization, failure analysis, product development support, and industrial troubleshooting, drawing on prior experience with organizations including Tetra Tech, FUCHS, BP Castrol, ENI, and TotalEnergies.

Author Contact Details

Dr. Raj Shah, Koehler Instrument Company
- Holtsville, NY11742 USA
- **Email: rshah@koehlerinstrument.com**
- **Web: www.koehlerinstrument.com**