AI/ML implementation in lubricants generation: challenges and prospects

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Abstract:

In recent years, the application of Artificial Intelligence (AI) in chemistry has become an active area of research. Earliest usage of AI in chemistry dated back to the 1960's, where this field was known as cheminformatics. An example of this early usage is the DENDRAL project developed at Stanford University. The field has grown during 1980's and 1990's where methods such as rule-based Machine Learning (ML) systems, clustering, artificial neural networks, and genetic algorithms became popular. Later on, with the development of new ML methods (especially deep learning), the availability of large amounts of data and the increase in computation power, AI and ML have become an important tool for chemistry applications.

Some common areas of AI application in chemistry include: molecular properties prediction, molecule design, retrosynthesis, reaction outcome and most famously drug discovery. However, with these applications come certain challenges and prospects.

This work explores the application of AI and ML in lubricants generation and especially in formulating Environmentally Acceptable Lubricants (EALs). It highlights the resultant prospects and challenges. Furthermore, it presents preliminary results for predicting toxicity, bioaccumulation, and biodegradability of EAL lubricants.

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