Artificial intelligence for formulating environmentally acceptable lubricants (EALs)

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Since November 2013, when Vessel General Permit (VGP) launched the regulation for vessels operating in the USA's coastal line, there has been an urgent need to develop EALs. A lubricant is considered environmentally acceptable if it complies with three main criteria, i.e. biodegradability, low toxicity to aquatic organisms, and non-bioaccumulation. Artificial intelligence brings a new approach to traditional lubricant formulation methods. This approach consists of mining in the diversity of ingredients and thus accelerating the lubricant formulation process since human abilities are limited and can be biased. This project has selected different databases to be mined such as EPA, ECHA, OASIS, etc. These databases are filtered and curated, and QSAR models are developed to build predictive models. Machine learning techniques used include RUSBoost, AdaBoost, Bagging, and ANN. So far, a simple model for bioaccumulation has been developed in this project. This model shows high accuracy in distinguishing between bioaccumulate and non-bioaccumulate chemical compounds.

Keywords: Environmentally acceptable lubricants; Vessel General Permit; machine learning; Artificial intelligence

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