QSAR optimization of engine lubricants at Lubrizol

Industry Sector

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QSAR

Researchers at Lubrizol (www.lubrizol.com) have used Quantitative Structure-Activity Relationships (QSAR) to study and optimize the performance of engine lubricants.

The techniques were used to predict the activities of new traction fluids, where other modeling techniques fail, and hence design new and improved lubricants. Published experimental tests were used to build the QSAR model, saving time and resources.

In order for toroidal transmissions to work effectively in engines, a traction fluid is required to lubricate the system. The most effective traction fluids require a high traction co-efficient to prevent slippage and hence get the best power transmission. Traction fluids are formulations with a base fluid and additives. The traction co-efficient is an inherent property of the base fluid but can be modified to enhance performance by additives such as anti-oxidants and dispersants.

Traction fluid coefficients are measured using a mini traction machine where the fluid is placed between a metal plate and ball and the coefficient is calculated. These are long tests to run, so minimizing the number of tests is important in controlling the time to develop a new traction fluid.

Using traditional modeling techniques such as quantum or classical mechanics on these systems would be challenging. Lubrizol used QSAR techniques to solve this problem.

QSAR generates a mathematical correlation, or model, between a known set of activity data, in this case the traction fluid coefficient, and a set of calculated descriptors. These descriptors can be as diverse as formulation data or molecular descriptors, such as the surface area of a molecule. Once a good model is developed, this is used to predict the activity for a new set of molecules.

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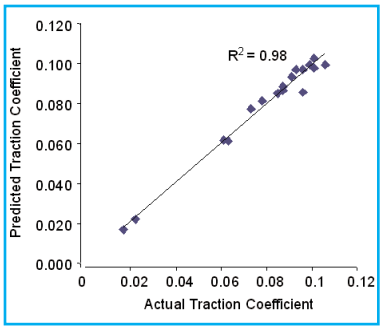
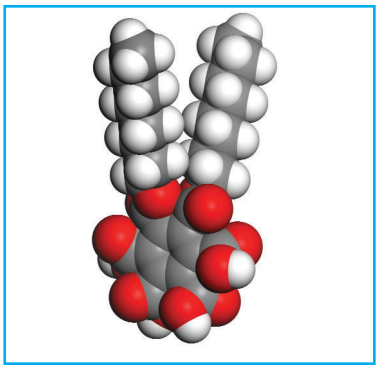
Previously published results[1] gave the values of the traction coefficient for twenty one molecules. These results were used by Lubrizol so they didn't have to run any tests before starting this work. These were partitioned into a training set, used to develop the model, and a test set of molecules. The test set is used to validate the model by answering the question, 'Will this model be predictive for molecules outside of the training set?'

Lubrizol used Accelrys' Genetic Function Approximation[2] (GFA) method to build predictive regression models. The GFA method is an evolutionary algorithm which uses natural selection techniques to pick the best descriptors. This is important, as the GFA will pick the few most important descriptors from a large selection.



▲ *Figure 1: The predicted against experimental traction coefficient values for the training set.*

Lubrizol used the GFA to generate several models with excellent r^2 and cross-validated r^2 values. The best equation, with an r^2 value of 0.98, contained the Jurs[3], Shadow Indices[4], and molecular refractivity[5] descriptors. These descriptors are all related to the shape and flexibility of molecules - features which the chemists intuitively felt were important in traction fluid design.



▲ *Figure 2: Molecule C, one of the three disparate molecules in the test set.*

The model was then used to predict the traction coefficient for the three molecules from the test set. The predicted and experimental values for these molecules were in very close agreement and are shown below.

	Molecule A	Molecule B	Molecule C
Predicted	0.100	0.050	0.077
Actual	0.100	0.050	0.076

References

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