Proposed Inclusive Model for the Prediction of the Derived Cetane Number (DCN) of Fuels Using Molecular Parameters

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According to the United States' Energy Information Administration (EIA), it is predicted that fossil fuels will power 77% of the global economy in 2040. The catastrophic impacts such fuels have on the environment necessitates the production of new clean and optimized fuels that will burn efficiently in engines. This project proposes an inclusive Multiple Linear Regression (MLR) model that will help in the production of fuels by predicting the Derived Cetane Number (DCN) - a measure of ignition quality - while avoiding experimental, expensive, and time/resource consuming standard methods. This model will facilitate assessment of fuels and help fuel developers chemically edit fuel mixtures to obtain desired ignition characteristics. Furthermore, it accurately predicts DCN values of oxygenated formulations with two common fuel additives, alcohol and ether, and is sensitive to hydrocarbon branching. The multivariate model is based on the extent of effect with eight structural parameters, molecular weight, and the Branching Index on DCN. This correlation was derived from a dataset consisting of 71 pure compounds and 137 blends of hydrocarbons (FACE gasolines, surrogate fuels). Experimentally measured DCN of 30 oxygenated surrogate/real gasoline blends were used to validate the prediction accuracy of the model. The predicted and actual DCN values of the tested blends matched well, with a 0.92 correlation coefficient upon comparison. In this regard, the proposed model has the potential to facilitate the fuel production process and allow for further application and creation of clean synthetic fuels.