Prediction of Autoignition Temperatures of Organic Compounds from Molecular Structure

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Quantitative structure-property relationship methods are used to develop mathematical models that predict autoignition temperatures (AIT) of organic compounds directly from molecular structure. Such models are developed with multiple linear regression analysis or with computational neural networks (CNN) from a training set of compounds with known AIT values. The 327 compounds and associated AIT data came from the CHEMSAFE database. The compounds are represented by calculated molecular structure descriptors that encode important structural features. The descriptors that are used in the final models are chosen by feature selection procedures that use either simulated annealing (SA) or the genetic algorithm (GA) coupled with either regression analysis, to generate linear models, or a computational neural network, to generate non-linear models. A number of models were generated for structurally-defined subsets of compounds, including high-temperature and low-temperature hydrocarbon models and models for oxygen- and nitrogen-containing compounds. The non-linear models found with the SA-CNN and GA-CNN approaches have root-mean-square errors for AIT prediction that are comparable to the experimental errors of the data. The details of the methodology used and the models found will be presented.