Methane Number model based on a Deep Neural Network

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The Methane Number, just as the Octane Number, provides an indication of knock propensity of a fuel. It is an important metric for manufacturers of reciprocating engines, as high efficiency, fuel flexibility and low emissions are highly desirable. However, the range of fuels, which customers are willing to utilize in the engines is increasing, i.e. due to an idea of energy storage in fuels (Power-to-Ammonia, Power-to-Hydrogen, etc). The motivation for this work is to extend widely available Methane Number calculators and enable assessment of knock propensity of new fuels, not present in the calculators. The Methane Number model is developed using a Deep Neural Network. The model takes as an input physicochemical properties of a mixture (e.g., ignition delay time and laminar burning velocity at certain condition, activation energy, molar mass) instead of a name of this mixture. In order to develop the model firstly an extensive dataset of methane numbers for variety of mixtures has been collected from the Cummins Fuel Quality Calculator. Secondly, each mixture has been characterized by its physicochemical properties, what created a final dataset used for training of the model. Ignition delay times, activation energies and laminar burning velocities were calculated with a detailed reaction mechanism: NUIG n-Heptane using Cantera in Matlab environment. The model was trained and tuned in R with the FCNN4R package. Validation performed on unseen fuels proves that the undertaken approach is robust, and the model is accurate.