

Laminar Flame Speed Modeling of Hydrogen, Methanol and Ammonia Using Machine Learning of Machine Learning

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ABSTRACT

Currently fossil fuels power almost all transportation. However, fossil fuels are responsible for significant levels of air pollution and global warming due to their high carbon content and resulting CO₂ emissions. The replacement of fossil fuels with low carbon fuels is one way to reduce CO₂ emissions from the transport sector. Hydrogen (H₂), methanol (CH₃OH), and ammonia (NH₃) are low or zero carbon fuel alternatives to the commonly used fossil fuels including gasoline and diesel. To develop these fuels for internal combustion engines, combustion models to analyze engine performance are needed. The laminar flame speed (LFS) is an essential attribute of a fuel-air mixture that is required for developing combustion models. LFS can only be experimentally measured for low temperatures and pressures compared to typical engine working pressures and temperatures. Combustion mechanisms used to calculate LFS for high pressure and temperatures are computationally expensive and not suitable for engine models that are used for engine control development.

In this study, LFS values are calculated by utilizing machine learning methods. To accomplish this, the LFS for hydrogen, methanol, and ammonia is calculated based on selected combustion mechanisms over the entire engine working condition pressures and temperatures. The created LFS simulation datasets include a collection of more than 160000 operating conditions from the combustion mechanism models. These datasets are then used to train Artificial Neural Network (ANN) and Support Vector Machine (SVM) models. With the aid of these machine learning techniques, it is possible to predict the LFS much more quickly than typical combustion mechanisms. The developed LFS models are also trained for fuel combinations using the LFS dataset of different fuels and blended fuels. For single fuels, the results show that ANN has better performance than SVM and can predict the LFS with a coefficient of determination R² value higher than 0.999. SVM is more efficient for a combination of fuel with R² values close to 0.99. Generally, both methods are well suited for modeling LFS for the three fuels, indicating that machine learning is capable of providing fast accurate models of LFS. The resulting LFS models can be integrated in an Engine Simulation Model to allow control development of these low carbon fuels in internal combustion engines.

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