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Development of Reduced Chemical Kinetic Models for the Numerical Simulation of Combustion and Emissions Behavior of Representative Conventional and Bio-Derived Fuels

Project 1910
June 2020

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The advancement of combustion technology through computer-aided development of novel combustion engines leads to cleaner and more efficient transportation systems. In these developments, numerical modeling, valued for its flexibility and low cost compared to experiments, is a powerful tool used for the prediction of combustion and emissions behavior of potential transportation fuels. However, two main challenges limit combustion simulations. Research requires different types of numerical models to simulate separate combustion problems, such as auto-ignition and flame propagation. Also, larger detailed models provide accurate predictions at the expense of time and computational resources. Addressing such challenges would lead to less time-consuming simultaneous simulation of different combustion problems without sacrificing accuracy.

Study Methods

To link auto-ignition and flame propagation behavior, researchers examined parametric dependence of flame time and ignition delay time using chemical kinetic models for methane, propane and ethanol. They developed a correlation between flame time and ignition delay time to enable the prediction of flame speed of a specific fuel from auto-ignition behavior. To address the model size challenge, researchers used the Stochastic Species Elimination (SSE) reduction approach, which excludes chemical species from the model based on their importance in the simulation of a combustion event, to reduce the size of a literature model for tetrahydrofuran (THF), a promising transportation biofuel, based on ignition delay time simulations at various pressures and temperatures. This research simulated ignition delay times using detailed and reduced models to compare the performance of such models. Researchers then identified the most important reactions responsible for the performance of the reduced model using sensitivity analysis. They then

updated reaction rates of such reactions to improve the agreement of reduced model predictions with literature of experimental ignition data.

Simultaneous flame propagation and auto-ignition behavior prediction is possible through correlating flame time with ignition delay time.

Findings

The parametric study showed that flame time and ignition delay time decrease with increasing temperature and pressure. Pressure more significantly influenced ignition delay time than did flame time. Both times decreased with more oxygen, with flame time having stronger dependence on the oxygen content than ignition delay time. A direct correlation between both times was developed for methane, indicating that slower flame propagation is linked to stronger auto-ignition resistance at the same condition. Compared with propane and ethanol, methane consistently exhibited slower flame propagation based on flame time calculations. Propane and ethanol generally exhibited similar flame propagation trends. SSE was used to develop a global reduced version of a literature detailed THF model at less than half the size. The reduced model tended to overestimate ignition delay times compared with the detailed model. Several reactions responsible for this deviation were identified by sensitivity analysis, including H-abstraction reactions from THF to produce reactive radicals. Their reaction rates were updated to increase their priority in the chain reaction. The modified version showed superior performance to the detailed model during ignition delay time simulations. It reproduced on experimental shock tube ignition data from the literature. This would lead to more accurate characterization of the combustion performance of THF, which can support its use as an additive or a pure fuel in transportation systems.

Policy Recommendations

Based on the findings of this research, a machine-learning based technique for the simultaneous simulation of flame and auto-ignition behavior can be developed to support turbulent combustion simulations. Also, SSE method can be modified to use flame time as the target event instead of ignition delay time to develop flame-focused reduced models. Accurate characterization of flame behavior of fuels can be of importance to firefighting agencies for instance. Finally, SSE can be used to develop models for the auto-ignition simulation of THF blends with conventional fuels since biofuels are mostly used as additives, since THF is more likely to be used as an additive to conventional fuels in the near future.

About the Author

Mazen A. Eldeeb is an Assistant Professor of Mechanical Engineering at California State University, Fresno. His main research interests are Biofuel Combustion and Chemical Kinetic Modeling.

To Learn More

For more details about the study, download the full report at transweb.sjsu.edu/research/1910

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