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Model Development and Analysis of Clean and Efficient Engine Combustion 2019 Annual Progress Report

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Disclaimer

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I.12 Model Development and Analysis of Clean and Efficient Engine Combustion (Lawrence Livermore National Laboratory)

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Project Introduction

Internal combustion engine design is increasingly driven by computational models used to predict performance metrics, which previously would have been predicted by limited design intuition or expensive and time-consuming physical testing. Improved model capabilities shorten design cycles and enable the production of cleaner and more efficient engines. This project focuses on advancing the state of the art in internal combustion engine simulations. The overarching goal is to enable predictive models and reduced time to solution for simulations that have impacts on combustion engine design.

Objectives

Overall Objective

- Advance the state of the art in engine simulation through development of fast and accurate models
- Work with industry partners to prove capability and impact of combustion software.

Fiscal Year 2019 Objectives

- Investigate the impact of reduced mechanisms on engine simulation results
- Develop fast solvers for one-dimensional diffusion flames
- Release Zero-Order Reaction Kinetics (Zero-RK) software as open-source.

Approach

This project is an ongoing research effort under the Advanced Combustion Engines subprogram, with annual feedback and direction from program managers and memorandum of understanding partners. During the current performance period, this project has focused on three areas: (1) exploring the impact of mechanism reduction on engine simulations, (2) creating new fast solvers for one-dimensional non-premixed flames, and (3) open-source release of the Zero-RK software package.

Results

Impact of Mechanism Reduction on Engine Simulations

Despite continued reduction in computational costs through work in this project and elsewhere, fully detailed reaction models containing thousands of species remain too expensive to include in many engine computational fluid dynamics (CFD) simulations. The constraints on model size result from the high grid resolution necessary in some cases to resolve fine flow structures, or from the short turn-around times required by industrial design cycles. To help understand the impact of mechanism reduction, the project team performed a study in the context of the Engine Combustion Network Spray A condition. Two complementary approaches to mechanism reduction have been developed to research the impact of reduction method and size on CFD simulation results. The first method leverages the directed relation graph (DRG) technique [1],[2] and incorporates the Zero-RK fast chemistry solver [3] to accelerate the process by an order of magnitude. This iterative method produces reaction models of varying size and accuracy. Figure I.12.1 compares mechanism size with the reduction accuracy threshold for reduction of an n-dodecane reaction model. Initially, many species can be removed with small error introduced. Subsequently, the amount of error introduced by further reduction rises quickly, and a plateau is seen at about 200 species, at which point further reduction leads to unacceptably large deviations between the reduced and the fully detailed models. For the current analysis, the smallest acceptable mechanism (with 219 chemical species) was used in the Spray A simulations and is referred to as the DRG mechanism.

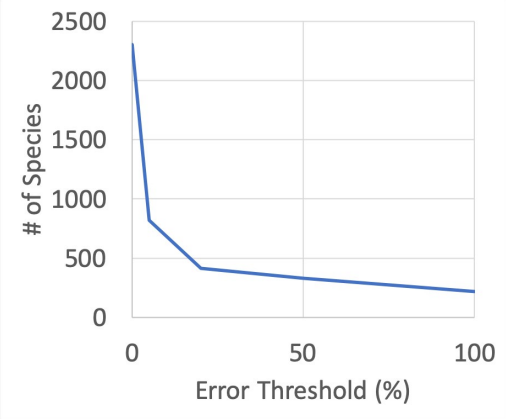


Figure I.12.1 Reduction process for the n-dodecane mechanism using the DRG method. Mechanism size in number of species is reduced according to an error threshold with respect to the fully detailed model.

The project also applied a separate hybrid approach [4] to the n-dodecane reaction model. Briefly, the hybrid model combines a detailed C0-C4 reaction model with a skeletal reaction model for the parent fuel, which is tuned to reproduce the results of the fully detailed mechanism. The hybrid methodology is able to predict the low- and high-temperature ignition with only 65 chemical species. Figure I.12.2 compares the ignition predictions for the full mechanism with the DRG and hybrid mechanisms as well as with the mechanism of Yao et al. [5] (a reduced mechanism that has been used in many reported studies of Spray A). Both of the new reductions capture the overall trend defined by the fully detailed mechanism, including the size and location of the so-called negative temperature coefficient regime. The hybrid mechanism does a slightly better job in matching the location of the extrema for the negative temperature coefficient regime for the first-stage ignition. The Yao mechanism is in worse agreement with the detailed mechanism than with both of the new reductions with respect to its predictions of longer delays at high and low temperatures and shorter ones in the negative temperature coefficient regime.

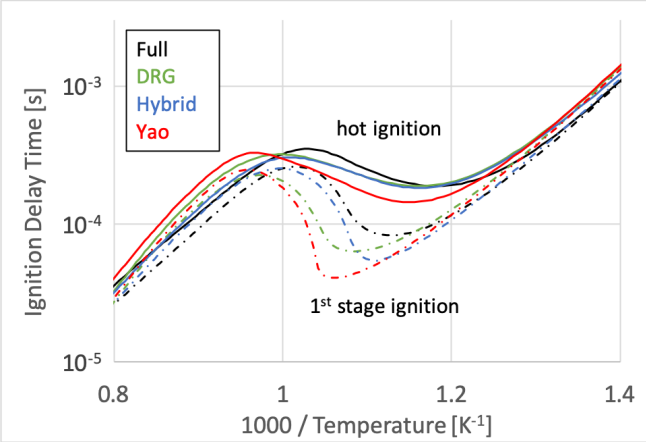


Figure I.12.2 Comparison of predicted ignition delay time as a function of inverse temperature for stoichiometric mixtures of n-dodecane and air at 6 MPa initial pressure for four reaction models

Both of the newly generated mechanisms were used in simulations of the Engine Combustion Network Spray A condition and compared with the fully detailed reaction model and the mechanism of Yao et al. The predicted ignition timings of the spray are shown in Figure I.12.3. All four tested mechanisms capture the overall trend from the experiments; however, the Yao mechanism does not predict ignition at the lowest ambient temperature (750 K). The exact chemical reasons for the differences in predictions are difficult to disentangle in these high-dimensional simulations. Figure I.12.4 shows the distribution of formaldehyde (a common indicator of low-temperature ignition) along a spray co-axial plane during ignition for each of the four mechanisms with ambient temperature set to 900 K. The Yao and hybrid mechanisms agree with the fully detailed mechanism with respect to the shape of the distribution; however, the Yao mechanism does not agree as closely in magnitude of the peak. The DRG mechanism predicts a different shape to the formaldehyde distribution. Based on these results, the project recommends the hybrid mechanism as a good compromise between model complexity/cost and accuracy for engine simulations. The overall comparison is possible because of the fast chemistry solvers for CFD that have been developed in this project [3], as they make the simulations incorporating the fully detailed mechanism feasible.

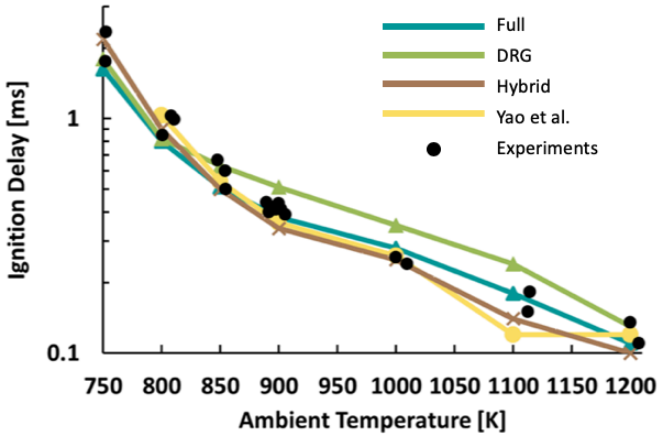


Figure I.12.3 Predicted and measured ignition time for spray combustion of n-dodecane at the Spray A condition as a function of temperature

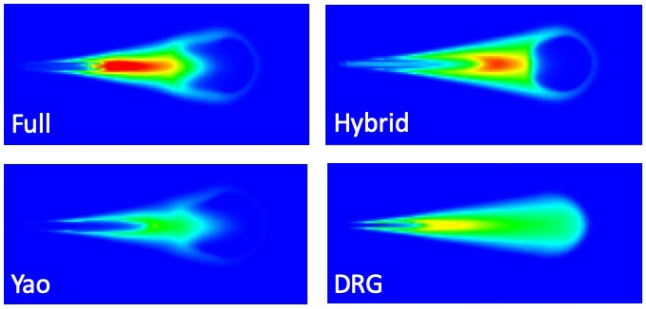


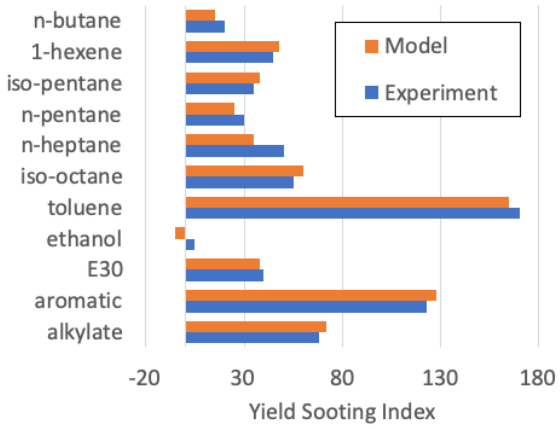
Figure I.12.4 Distribution of formaldehyde over spray co-axial plane during first-stage ignition of n-dodecane at Spray A condition (900 K), compared for four reaction models

Diffusion Flame Solvers for Flamelet Simulations

Simulations of one-dimensional combustion systems using detailed kinetics have many important applications in the study of boosted spark-ignited and multi-mode engine configurations. Premixed flame simulations can be used to generate flame speed correlations used in the study of knock, while non-pre-mixed flames capture important dynamics relevant to multi-mode engines in which the operating regime can transition between well-mixed and diffusion-dominated combustion.

The project has developed fast solvers for simulation of the flamelet equations for non-pre-mixed (or diffusion) flames that are orders of magnitude faster than previously available tools. The flamelet solver extends ideas developed previously in this project [6] to the new non-pre-mixed context and applies a novel numerical technique to reduce the computational cost of solution while maintaining accuracy. Briefly, the method uses an iterative approach, preconditioned by an approximate Jacobian matrix that is factorized into two components (related to chemistry and transport), which can each be further processed efficiently because of the sparsity of each. The resulting simulation cost (in wall time) scales linearly with the number of chemical species included. The linear scaling translates to multiple orders of magnitude reduction in simulation time for mechanisms with greater than 1,000 species when compared with competing solutions such as FlameMaster [7]. Both steady and unsteady solvers have been developed and include central processing unit (CPU) parallelization to further reduce time to solution.

The fast flamelet solver makes it possible to do analyses that were too expensive with previous tools. One of the first applications is investigating the chemical drivers of soot production. The solver has been adapted to predict yield sooting indexes based on the work of Xuan and Blanquart [8]. Figure I.12.5 shows a validation of the solver applied to yield sooting index prediction for a variety of engine-relevant fuels compared with experimental measurements [9]. After validation, the project team applied the solver to computing the sensitivity of soot production to individual reaction rates. This computation requires a solution of the steady flamelet equations for each reaction in the model (of which there can be tens of thousands). It is estimated that FlameMaster (one of the only existing tools for this type of analysis) would require more than 20,000 CPU hours for this computation, while the new fast flamelet solver required only 33 CPU hours. The project team is analyzing the reaction sensitivities in collaboration with Professor Xuan at The Pennsylvania State University. The results will be submitted for publication.



E30 – blend of 30% ethanol with gasoline

Figure I.12.5 Comparison of measured yield sooting index with those predicted with the fast flamelet solver (experimental data from McEnally et al. [9])

Zero-RK Code Release

The Zero-RK fast chemistry solvers developed in this project have significantly improved time to solution for many engine simulation scenarios. However, previously, the tools were limited in use to LLNL researchers and collaborators. The work of these researchers has produced a good set of results in the form of refereed research publications [10],[11],[12],[13],[14] but Zero-RK was not available to industry for direct application to organizations' internal research and design processes. With the help of the Industrial Partnerships Office at LLNL, the Zero-RK code has been released as an open-source package available with a permissive license to combustion researchers throughout the world. The package is available on LLNL's github page (https://github.com/LLNL/zero-rk) and contains the code necessary to run constant-volume, well-stirred reactor models and an interface to couple with reacting flow CFD codes. The wide availability of the code will greatly broaden the impact of the Zero-RK tools on industry problems. Further code releases are planned to include a variable-volume application, flame solvers, and other future developments in this program.

Conclusions

- Developed new understanding of the impact of mechanism reduction on engine CFD and recommended a hybrid approach for mechanism reduction as the best tradeoff between mechanism complexity and accuracy
- Created new fast solvers for one-dimensional diffusion (flamelet) flames that are 10–100 times faster than previous methods and can be used to generate tabulated chemistry for engine CFD and to investigate sensitivity of soot production to chemical reactions
- Released Zero-RK fast chemistry solver as free and open-source software.

Key Publications

1. Lapointe, S., R.A. Whitesides, and M.J. McNenly. 2019. "Sparse, Iterative Simulation Methods for One-Dimensional Laminar Flames." *Combustion and Flame* 204: 23–32. https://doi.org/10.1016/j.combustflame.2019.02.030.

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10. Lapointe, S., C.L. Druzgalski, and M.J. McNenly. 2018. "Numerical Study of a Micro Flow Reactor at Engine Pressures: Flames with Repetitive Extinction and Ignition and Simulations with a Reduced Chemical Model." *Combustion and Flame* 197: 102–110. https://doi.org/10.1016/j.combustflame.2018.07.020.

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