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Zero-RK Acceleration of Low-Life-cycle Carbon Fuel (LLFC)Simulations

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Disclaimer

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V Crosscutting

V.1 Zero-RK Acceleration of Low-Life-cycle Carbon Fuel (LLFC) Simulations (Lawrence Livermore National Laboratory)

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Project Introduction

Designing modern combustion systems now relies on computer models that predict how changes in design will affect performance. These models have replaced older methods that relied on the designer's intuition or costly and time-consuming physical testing. By using improved models, design cycles can be shortened and cleaner and more efficient combustion devices can be created. This project aims to improve computer simulations of low-life-cycle carbon fuels (LLCFs) with the goal of making these simulations faster and more accurate for predicting combustion in vehicles.

Objectives

Overall Objectives

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

Fiscal Year 2023 Objectives

- Create surrogates for renewable diesel and conventional aviation fuels to be utilized by partners in the Decarbonization of Off-road, Rail, Marine, and Aviation (DORMA) program.
- Develop Heterogeneous-compute Interface for Portability (HIP) version of Zero-RK graphics processing unit (GPU) solvers to enable fast solution of chemical source terms on Advanced Micro Devices, Inc. (AMD)-based compute platforms such as Frontier at Oak Ridge National Laboratory (ORNL) and El Capitan at Lawrence Livermore National Laboratory (LLNL).

Approach

Computational models are critical for the transition of U.S. transportation networks of off-road, rail, marine, and aviation away from carbon-intensive fuels (e.g., diesel and Jet-A/A1) to LLCFs. These models rely on detailed chemical kinetics to capture ignition, propagation, extinction, and emissions behavior as a function of fuel composition. Implementation of these models requires fuel models that mimic the physical and chemical properties of market fuels (which, in general, are too complex to match component-by-component in models) and efficient methods of incorporating the detailed reaction kinetics into relevant simulations. The current effort in this project has closed gaps in these areas by (1) creating new fuel surrogates for two fuels relevant to off-road, marine, and aviation combustion and (2) extending the current capability to utilize GPU hardware for

fast solution of chemical source terms in computational fluid dynamics (CFD) simulations to new architectures being fielded in U.S. Department of Energy (DOE) supercomputers as well as industry high-performance computing (HPC) centers.

Results

Fuel Surrogates for DORMA Research

Petroleum-derived market fuels used in transportation (e.g., diesel and jet fuels) contain thousands of components that can vary seasonally and from region to region. The complexity of these fuels necessitates the use of surrogate blends that match the physical and chemical qualities of a targeted fuel with a limited mixture of well-characterized fuel components. LLNL has developed tools for generating such blends that have previously yielded surrogates proven to match real fuel characteristics and performance with high fidelity [1]. In the current performance period, these tools have been applied to the generation of two novel surrogates, one for a renewable diesel blend and another for a research jet fuel.

The renewable diesel surrogate was generated in partnership with ORNL and principal investigator Flavio Chuahy. ORNL supplied target properties for a candidate renewable diesel as well as a palette of potential surrogate components selected due to their inclusion in the chemical reaction model being used in the simulation studies. The data include derived cetane number (DCN), liquid density, percentages of linear and branched alkanes, carbon number distribution, and distillation curve. LLNL worked iteratively with ORNL to create a suitable surrogate for use in ORNL's study, which determined optimal operating conditions for conventional and renewable diesels. The chosen surrogate was able to provide a good match to all the targeted properties except for the ratio of linear-to-branched alkanes. For the fuel components available in the reaction model, it was necessary to choose between good agreement with DCN or the molecular classes. DCN was favored as being more important to model predictions. Figure V.1.1 and Figure V.1.2 show the distillation and carbon number data for the target fuel and surrogate fuel, and Table V.1.1 provides details on the other targeted quantities for the renewable diesel and the surrogate. Future studies may examine the importance of matching compositional and other properties with more detailed reaction models containing more fuel components.

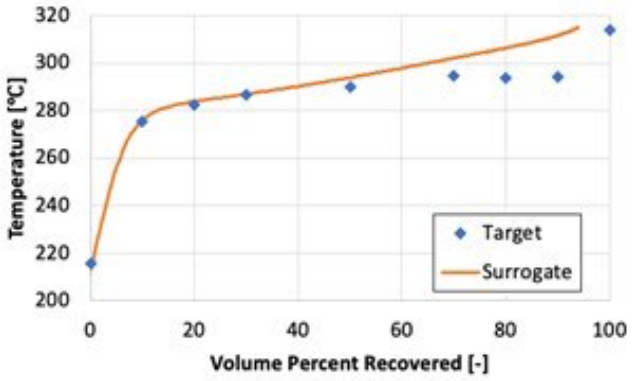

Figure V.1.1 Measured and predicted distillation curve for renewable diesel fuel and proposed surrogate, respectively

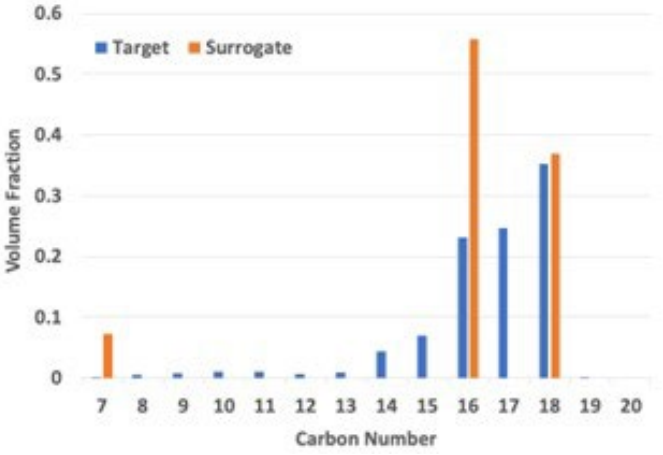

Figure V.1.2 Carbon number distribution for target renewable diesel fuel and proposed surrogate

Table V.1.1 Target and Surrogate Properties for Renewable Diesel Fuel

Property Target	Target Value	Surrogate Value
DCN	80.7	80.48
Density [kg/m³]	0.775	0.766
n-alkane volume %	0.13	0.784

The aviation fuel surrogate was produced as a starting point for high-fidelity reaction modeling of conventional and sustainable aviation fuels. The target fuel is designated as POSF 10325, a well-characterized, experimental fuel created as part of the National Jet Fuel Combustion Program with the intent of being representative of typical properties of current petroleum-derived jet fuels. While many previous surrogates have been proposed for this fuel, none have been able to take advantage of advances in recent reaction models to be able to simultaneously match volatility, ignition, and emissions behavior of the fuel. The fuel properties of DCN, molecular weight, density, hydrogen-to-carbon ratio, and detailed compositional data were reported by Edwards [2], the advanced distillation curve by Saggese et al. [3], and the yield sooting index (YSI) by Das et al. [4]. Leveraging the comprehensive reaction model developed at LLNL under a sister project [5], 32 fuel components were selected as the initial palette to match these targets. This broad palette provides great flexibility in matching the targeted properties, but a 32-component surrogate is unattractive from both a modeling and experimental perspective and so a sparsity enhancing target was also included during the surrogate optimization process. The result of the optimization is a nine-component surrogate fuel that provides good agreement with all of the targeted properties (see Table V.1.2 and Figure V.1.3).

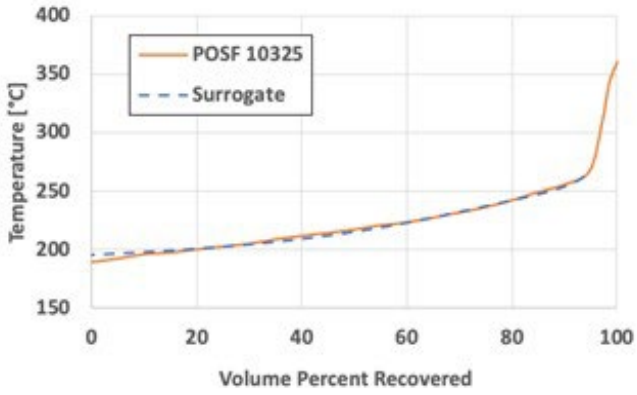

Figure V.1.3 Measured and predicted distillation curve for conventional jet fuel and proposed surrogate, respectively

Table V.1.2 Target and Surrogate Properties for POSF 10325 Jet Fuel

Property Target	Target Value	Surrogate Value
DCN	48.3	48.29
Density [kg/m³]	0.803	0.795
Hydrogen:Carbon Ratio	1.94	1.92
Molecular Weight	159	158.8
YSI	70.3	70.27
n-alkane vol%	0.212	0.218
iso-alkane vol%	0.315	0.321
monocyclo-alkane vol%	0.246	0.239
Dicyclo-alkane vol%	0.06	0.051
Total aromatic vol%	0.165	0.159
Diaromatic vol%	0.018	0.0118
Cyclo-aromatic vol%	0.028	0.0126

Heterogeneous-Compute Interface for Portability Version of Zero-RK GPU

State-of-the-art combustion research utilizing detailed CFD continues to be constrained by available computational resources. The computing hardware landscape has evolved in recent years to be highly dependent on GPU technology at the leading edge of performance in terms of total floating point operations (FLOPs) and FLOPs per watt as cataloged in the TOP500 list of supercomputer performance [6]. In past reports, this project has detailed work done to enable acceleration of combustion simulations on GPU hardware developed by the NVIDIA Corporation, which has historically been the majority hardware vendor, especially at DOE facilities. In recent years, GPUs produced by AMD have become more relevant and have prompted the development of a new version of the Zero-RK solver that can run on these systems.

In the current performance period, a new version of the Zero-RK solvers has been developed for AMD GPUs. The work started by leveraging tools provided by AMD to semi-automatically convert the existing Compute Unified Device Architecture code to the HIP code. Development was performed on the El Capitan early access platforms at LLNL. After the initial conversion process, significant effort was required to ensure that the code could be built reliably on the relevant platforms. Finally, work is continuing to improve performance for industry-relevant simulation conditions.

Conclusions

- Two novel fuel surrogates relevant to current and future LLCF research have been developed and are being used by DORMA projects.
- A new implementation of GPU-accelerated chemical kinetics solvers targeting AMD hardware has been created and will be deployed at DOE and industry HPC sites.

Key Publications

1. Assanis, Dimitris, Gaurav Guleria, Joonsik Hwang, Dario Lopez Pintor, Scott Wagnon, and Russell Whitesides. 2023. “Quantitative Validation of a Computational Fluid Dynamics Methodology for Gasoline Sprays under Cold Start Conditions.” SAE Technical Paper. Warrendale, PA: SAE International, April 11. https://www.sae.org/publications/technical-papers/content/2023-01-0300/.

2. Kukkadapu, Goutham, Russell Whitesides, Mengyuan Wang, Scott W. Wagnon, Marco Mehl, Charles K. Westbrook, Robert McCormick, Chih-Jen Sung, and William J. Pitz. 2023. “Development of a Diesel Surrogate for Improved Autoignition Prediction: Methodology and Detailed Chemical Kinetic Modeling.” *Applications in Energy and Combustion Science* 16 (December 1): 100216. https://doi.org/10.1016/j.jaecs.2023.100216.

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1. Cheng, Song, S. Scott Goldsborough, Scott W. Wagnon, Russell Whitesides, Matthew McNenly, William J. Pitz, Dario Lopez-Pintor, and John E. Dec. 2022. “Replicating HCCI-like Autoignition Behavior: What Gasoline Surrogate Fidelity Is Needed?” *Applications in Energy and Combustion Science* 12 (December 1): 100091. https://doi.org/10.1016/j.jaecs.2022.100091.

2. Edwards, James T. 2017. “Reference Jet Fuels for Combustion Testing.” In 55th AIAA Aerospace Sciences Meeting. AIAA SciTech Forum. American Institute of Aeronautics and Astronautics. https://doi.org/10.2514/6.2017-0146.

3. Saggese, Chiara, Ajay V. Singh, Xin Xue, Carson Chu, Mohammad Reza Kholghy, Tongfeng Zhang, Joaquin Camacho, et al. 2019. “The Distillation Curve and Sooting Propensity of a Typical Jet Fuel.” *Fuel* 235 (January 1): 350–62. https://doi.org/10.1016/j.fuel.2018.07.099.

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Fuels, and Their Surrogates in Diffusion Flames." *Fuel* 197 (June 1): 445–58. https://doi.org/10.1016/j.fuel.2017.01.099.

5. Wagnon, S.W. 2023. "LLCF Combustion and Emissions Models." *Decarbonization of Off-Road, Rail, Marine, and Aviation Program: 2023 Annual Progress Report*. U.S. Department of Energy, Washington, DC.

6. Dongarra, Jack, and Piotr Luszczek. 2011. "TOP500." *Encyclopedia of Parallel Computing*, edited by David Padua, 2055–57. Boston, MA: Springer US. https://doi.org/10.1007/978-0-387-09766-4_157.

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LLNL Document Number: LLNL-TR-XXXXXX