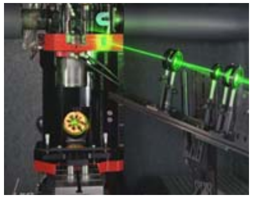
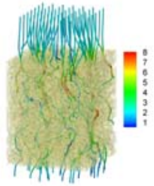
EXPLORE AND COLLABORATE
AMERICAN INDUSTRY AND AMERICA'S NATIONAL LABS
MATERIALS FOR ENERGY APPLICATIONS

CLEAN AND EFFICIENT COMBUSTION FOR ENERGY SECURITY

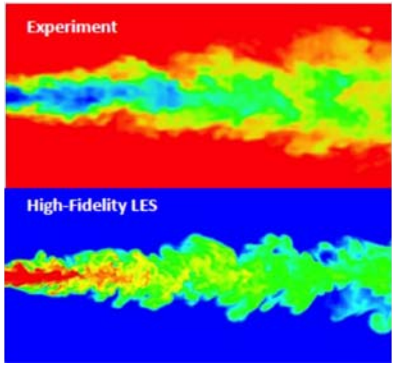
Partnerships for American Competitiveness

Increasing the efficiency of internal combustion engines is a technologically proven and cost effective approach to dramatically improving the fuel economy of the nation's fleet of vehicles in the near- to mid-term, with the corresponding benefits of reducing our dependence on foreign oil and reducing carbon emissions. Achievable advances in engine technology can improve the fuel economy of automobiles by over 50% and trucks by over 30%. Increased turbine efficiency will also assist power generators to meet regulatory and market driven goals.





The national laboratories conduct research and development on all aspects of commercial combustion systems with the overall goal of enabling US industry to create clean and efficient systems that are economically competitive. This work spans internal combustion engines (left), exhaust gas after treatment systems (center) and turbine power generation (right). Close partnerships with industry help guide these programs to maximize their impact.



Cutting edge computation tools, such as large eddy simulation (LES), utilizing the latest massively parallel computers allow high-fidelity simulation of combustion under realistic conditions of temperature and pressure. Shown here is a simulation of turbulent jet flame. Note that the experiment lacks the resolution to reveal the complex flow structures present.

Predictive Simulation for Next-Generation Combustor Design

Timely realization of ambitious goals in combustion efficiency while meeting regulatory requirements will require industry to shrink its product development cycle. Current design processes, using "build and test" prototype engineering, will not suffice. Current market penetration of technologies is simply too slow – it must be dramatically accelerated.

These challenges present a unique opportunity to marshal U.S. leadership in science-based simulation to develop predictive computational design tools for use by the transportation industry. The use of predictive simulation tools for enhancing combustion engine performance will shrink engine development timescales, accelerate time to market, reduce development costs, while ensuring the timely achievement of energy security and emissions targets, and enhancing U.S. industrial competitiveness.

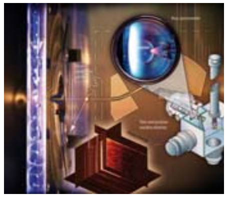
Combustion Science Foundation

Predictive simulation of combustion relies on thorough understanding of the relevant fundamental science underpinning turbulent combustion. Work is carried out in three broad areas: chemistry of combustion, light/matter interactions relevant to diagnostic development, and turbulent reacting flows.

Combustion chemistry studies encompass both theoretical and experimental investigations. Theory ranges from the development and application of ab initio methods for the calculation of molecular potential energy surfaces to the calculation of reaction rates. Experimental studies include investigation of individual molecular scattering events, measurement of reaction rates, and discovery of new chemical phenomena relevant to combustion.

The experimental investigation of combustion relies heavily on optical diagnostic methods to probe the simultaneously hostile and easily perturbed environments. The application of these methods in the complex combustion environment requires an understanding of both the light matter interactions as well as competing physical and chemical processes.

Turbulent reacting flow research focuses on the coupling of turbulence and chemistry that creates significant challenges for predictive modeling. Direct numerical simulation and high-fidelity large eddy simulation are the leading computational tools while laser-based methods are used to probe the chemical and physical structures of flames for validation of computations and discovery of new processes.



Sandia, Argonne and Lawrence Berkeley National Laboratories have collaborated on a project to unravel the complex chemistry of combustion through the use of synchrotron-based vacuum ultra-violet ionization mass spectrometry. The chemical reaction rates and mechanisms revealed through this work will allow combustor designers to accurately model efficiency and emissions.

Advanced Engine Combustion

The Advanced Engine Combustion (AEC) Memorandum of Understanding (MOU) establishes an understanding among the member partners concerning overall research directions and the management of the MOU. The MOU is focused on providing the science base needed to develop the next-generation of high-efficiency, clean engines for future fuels. Advanced low-temperature combustion (e.g., HCCI), lean-burn spark-ignition combustion, and advanced diesel combustion strategies are considered. Engines using these combustion strategies offer the potential for achieving significantly higher efficiencies and lower engine-out emissions than current engines on the road. Fuels considered in the research include conventional petroleum-based fuels, non-petroleum-based fuels (e.g., bio and synthetic fuels) and hydrogen.

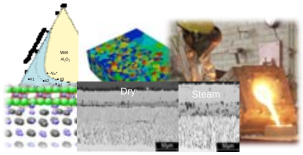
The AEC MOU participants include ten engine companies (General Motors, Ford, Chrysler, Caterpillar, Cummins, Detroit Diesel, John Deere, Navistar, Volvo, and General Electric), five energy companies (Chevron, ExxonMobil, ConocoPhillips, BP, and Shell), and six national laboratories funded by the DOE Office of Vehicle Technologies (Lawrence Livermore, Los Alamos, Oak Ridge, Argonne, Sandia, and the National Renewable Energy Laboratory).

The MOU is organized and led by Sandia National Laboratories. Industry partners are expected actively participate in the MOU. They attend the biannual MOU working group meetings (one held at Sandia and one held at USCAR); provide constructive feedback on research progress and directions at the national labs; make presentations on industry needs, perspectives and non-proprietary in-house research; and at their discretion, provide technical assistance and hardware to facilitate research at the national laboratories. For new partners to join the MOU, unanimous approval of the existing partners is required.

Combustion for Power Generation

The combustion of carbon based fuels dominates the National power production portfolio, and includes the air-based combustion, oxygen-based combustion, and partial oxidation of coal, natural gas, biomass and municipal wastes. The National Laboratory complex is utilizing an "Integrated Materials Development " approach, leveraging complementary experimental and computational approaches, ranging from the atomistic design of materials through the techno-economic assessment of combustion processes, all focused on increasing the efficiency (durability, life, etc.), decreasing the environmental impact (greenhouse gases, criterion pollutants, etc.) and accelerating the deployment of current and future combustion technologies.

Efforts are focused on designing and developing engineered materials tailored for a variety of current and emerging combustion technologies, including the oxy-combustion , chemical looping combustion, and advanced steam cycles and other novel working fluids. Research and development is specifically aimed at coupling advanced computational approaches for materials design and optimization with focused experiments on processing of materials and evolution of materials at scales and environments of industrial relevance.



The National Laboratory complex, in collaboration with industry, is focused on leveraging the capabilities and competencies at the scales necessary to overcome the technical challenges at hand.

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