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Provide for the science-based design tools necessary for industry to reduce CO_2 and petroleum footprint of the transportation fleet by 25%

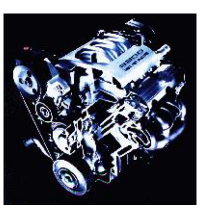
Transportation accounts for ⅔ of the nation's oil use and ¼ of its greenhouse gas (GHG) emissions. Aggressive national goals to reduce petroleum use by 25% by 2020 and GHG emissions by 80% by 2050 require major improvements in all aspects of America's energy use. To maintain our accustomed mobility, we must make the internal combustion engine more efficient while incorporating advanced, low-net-carbon fuels and other advances such as plug-in hybrid technologies to reduce petroleum imports and enhance U.S. industry competiveness.

The Combustion Research Facility at Sandia's California site.

Goals for 2050 may seem a long way off, but the automobile fleet turns over approximately every 20 years—every car sold in the U.S. in 2030 must meet the 80% CO_2 reduction—and implementing new technology takes ~15 years. So, technologies ubiquitous on 2030 vehicles must debut by ~2015. Fuels will also evolve, adding more complexity and further highlighting the need for efficient product-development cycles.

To meet this challenge the U.S. must marshal supercomputing and public–private partnership resources to develop predictive computational design tools for transportation industry use—to enhance engine performance and reduce development timescales, accelerate time to market, and reduce development costs, while ensuring the timely achievement of energy security and emissions targets.

Sandia's Combustion Research Facility (CRF) and modeling and simulation researchers collaborated with Cummins on their newest diesel engine—marketed in 2007 solely with computer modeling and analysis tools. Cummins reduced development time/cost by ~15% as they achieved a more robust design, improved mileage, and met all environmental and customer constraints.



Cummins 2007 diesel engine, developed with high-performance modeling and a fundamental knowledge of diesel combustion developed at the CRF.

The CRF's engine combustion research led the development of the science and technology (S&T) foundation for diesel combustion—a more than 15-year research effort, largely funded by DOE. Laser diagnostics in the CRF's optical engine facilities provided much of the detailed understanding of the physical and chemical processes that drive the very complex diesel combustion process. Other key contributors included Los Alamos and Lawrence Livermore national labs, and the universities of Wisconsin and Michigan.

Using this hard-won fundamental knowledge of combustion processes in conjunction with high-performance computing modeling and simulation, CRF researchers are now studying new, clean combustion strategies for high-efficiency engines utilizing future fuels.

Progress toward national petroleum and emission reduction goals can also be met through electric/hybrid vehicles. However, current battery technology imposes mobility limitations consumers are reluctant to accept. Sandia researchers are working to create a science-based understanding of the atomic/molecular processes and connect them with the macroscopic response of packaged batteries to mitigate safety concerns, extend battery lifetimes, and increase battery efficiency through three highly coordinated thrusts: large-scale battery testing (measure critical end-of-life mechanisms); *in situ* nano-scale characterization (atomistic understanding of these mechanisms); and multi-scale modeling (predictive models linking atomistic processes with macroscopic responses). These three thrusts, working in conjunction with materials and systems from industry partners, will enable predictive simulations of battery performance so critically needed to increase the capacity, lifetime, and safety of these new materials.

A nanowire battery before (top) and after (bottom) charging: 90% elongation, 35% diameter expansion, 250% volume increase.

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