PROGRAM facts

U.S. DEPARTMENT OF ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Ultraclean Fuels
Focus Area

06/2000

ULTRACLEAN FUELS SCIENCE AND TECHNOLOGY FOCUS AREA

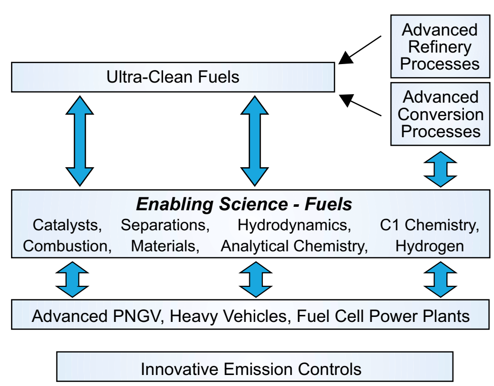
Background

The availability of a clean, stable and affordable energy supply for transportation is essential for sustaining economic growth, social stability, and public health. However, there are domestic and international concerns regarding transportation energy usage.

Over the next several years, the U.S. will implement stricter Federal and state clean air requirements for highway vehicles; encounter more volatile global energy markets; face increased economic competition in the international market for clean highway vehicle and fuels production technologies; and confront the threat of global climate change. Given this emerging situation, the research and development of advanced technologies for high-efficiency, low-emissions highway vehicles, as well as the production of ultraclean fuels required for their operation must be pursued. The R&D needs to address a broad range of feedstocks, including petroleum, natural gas, coal, refinery by-products, waste materials and renewable materials to enhance our resource base.

Description

The goal of the Ultraclean Fuels Focus Area initiative is to assist all elements of the U.S. refining and transportation industries to eliminate concerns associated with developing and introducing the alternative fuels necessary to meet the requirements of ultra-low emissions vehicles. The Department of Energy has created a strategic alliance among its fuels programs focusing on a common vision: "Partner with the U.S. energy industry to meet the growing demand for cleaner transportation fuels." To achieve this vision, a systems approach that complements the R&D being performed on advanced engines and emissions controls must be conducted. In addition, the program must incorporate projects that address both near- and long-term emission reduction targets.



Industry-led teams will be directed to perform systems-oriented R&D of fuel technologies that are ready to move beyond the laboratory. This R&D will focus on technologies used to produce a specific fuel from selected fossil feedstock, alone or in combination with other hydrocarbon materials. These projects will produce fuels in quantities sufficient for validating fuel quality, vehicle performance and emissions reductions. The program will support enabling R&D performed with industry direction at academic institutions and Department of Energy's national laboratories.

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NETL

Develop the enabling science for producing ultra-clean and affordable fuels for high-efficiency transportation systems.

At the Department of Energy (DOE), we are utilizing the unique scientific capabilities of our national laboratories and partnering with industry to identify, study, and develop advanced fuels for tomorrow's vehicles.

The DOE is already providing the Federal government's largest technology R&D contribution to the government/industry Partnership for a New Generation of Vehicles and is collaborating with the heavy-vehicle industry to develop high-efficiency truck technologies.

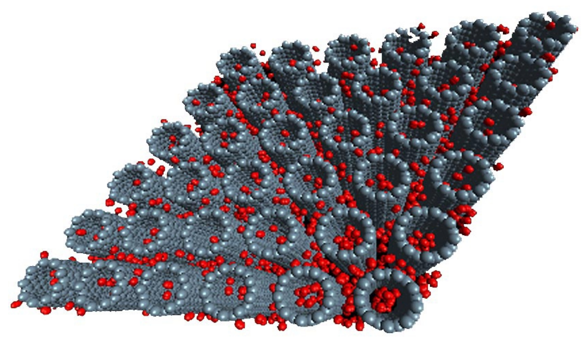
If we are to achieve the optimum combination of low emissions, high performance, long-term durability and affordability, it is essential that a systems approach be employed to address technology integration issues.

Scientific Challenges

There are three components to ultraclean transportation systems: ultraclean fuels, advanced engines, and emission control systems. Integrated development of these components is necessary to meet the criteria of high performance, ultralow emissions, long-term durability, and affordability. More specifically, developing and producing ultraclean fuels means addressing scientific challenges and advancing the state-of-the-art in a number of areas. These areas include Computational Chemistry, Novel Pathways to Low-sulfur Fuels, Advanced Analytical Techniques, Improvements in Separation Science, and Novel Synthesis Routes.

Computational Chemistry

Advances in high-speed computing and improved understanding of chemical structures have led to increased use of molecular modeling as a predictive tool for research in chemistry. Applying these methods to processes that use catalysts is particularly challenging, but has enormous promise. As a result, the Ultraclean Fuels Focus Area will investigate the use of computational science to improve the Fischer-Tropsch (F-T) process, hydrogenation, heteroatom removal, and hydrogen interactions with surfaces. The work will be conducted in collaboration with the University of Pittsburgh, Carnegie Mellon University, and Sandia National Laboratory.



Using computer models does not replace the need for experimental data, but rather, it changes the nature of the data required. As computation models become more sophisti-cated, the input data becomes more fundamental. For example, adjustable "lumped" parameter sets are replaced with rate constants for individual compounds undergoing specific reaction steps. In some cases, such data is available in the literature, while in others; experimental measurements will be required. The development of more advanced models will drive the need for better experimental data to support the models. In an iterative approach, experimental data will also be necessary to test and improve the model.

Novel Pathways to Low-sulfur Fuels

Strategies are needed to produce ultraclean fuels with very low sulfur levels, while at the same time maintaining fuel quality (e.g., octane number) and cost. Both classical (hydrogenation), as well as novel (non-reductive) approaches for heteroatom removal will be investigated.

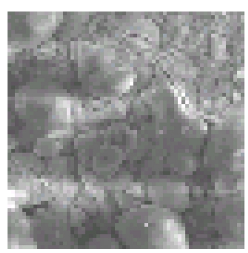
Classical hydrogenation involves the developing and using improved catalysts and processing schemes to hydrogenate sulfur moieties. Progress

is still being made in this regime, but the classical approach suffers from thermodynamic and kinetic limitations. For example, removing the sulfur from an aromatic ring requires that the entire ring be hydrogenated before the sulfur atom undergoes reaction. Since most refinery operations already operate in a hydrogen deficient environment, this is not an efficient use of valuable hydrogen. NETL, in collaboration with Carnegie Mellon University is evaluating an alternative, and promising, approach using selective oxidation with "green" catalysts. In this approach, the sulfur group is first "marked" by reaction with a peroxide catalyst specific to sulfur. A second step then eliminates the sulfur while leaving the remainder of the molecule unaffected.

Advanced Analytical Techniques

New and advanced analytical techniques will be necessary to characterize sulfur compounds at near-zero levels. A significant need will be develop technique that determines the specific sulfur compounds that exist at low levels. While sulfur detection itself is not expected to be an issue, as currently available techniques are capable of detecting sulfur in the part-per-billion range, speciation may be an issue. As regulations drive sulfur content to lower levels, removal technologies will have to target specific classes of sulfur compounds. Advanced analytical chemistry approaches to sulfur speciation may lead to developing processes for its removal.

In addition, there is a need to develop novel analytical techniques to characterize ultraclean fuels themselves. While the next generation of ultraclean fuels is being designed to fit the current transportation infrastructure, they may not be well described by traditional petroleum characterization methods. In such cases, new techniques will be needed for the determination and analysis of the critical properties.



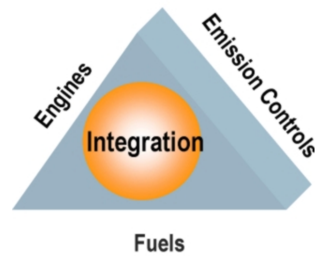
Improvements in Separation Science

The Focus Area will include research on advanced hydrogen separation and storage methodologies, as well as hydrogen production via reforming. A unique research facility at NETL will be used to investigate high-pressure, high-temperature hydrogen separation membranes, and safe hydrogen storage technologies. Collaborative research with Argonne National Laboratory and regional universities in advanced separation technologies and materials production will also be conducted.

Hydrogen can be produced from natural gas or other fossil feedstocks. However, improvements in current methods for hydrogen separation from other gases remains a key issue for large-scale production of hydrogen (as in a refinery or

System Requirements

- Ultra-low emissions
- High performance
- Long-term durability
- Low toxicity
- Affordability



The integrated development of all three components - - Fuels, Engines, and Emission Controls - - is necessary to produce ultra-clean transportation systems that will have high performance with ultra-low emissions, long term durability, low toxicity and are affordable.

In addition to reciprocating engines, there is also industry interest in the use of fuel cells for transportation applications.

Fuel cells presently depend on hydrogen as an energy source; therefore, the development of fuels that can easily be converted to hydrogen, and/or the affordable production and storage of hydrogen are needed.

Ultraclean Fuels Science and Technology Focus Area

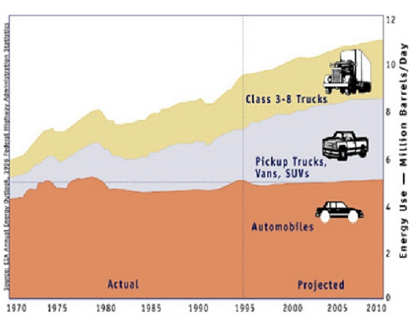
Research Drivers

Environmental Quality:
Vehicles are rapidly being regulated to low levels of emissions

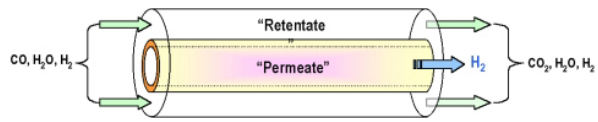
Global Climate Change:
The transportation sector generates 35% of the nations greenhouse gas emissions.

Energy Security:
The transportation sector is heavily dependent on imported petroleum.

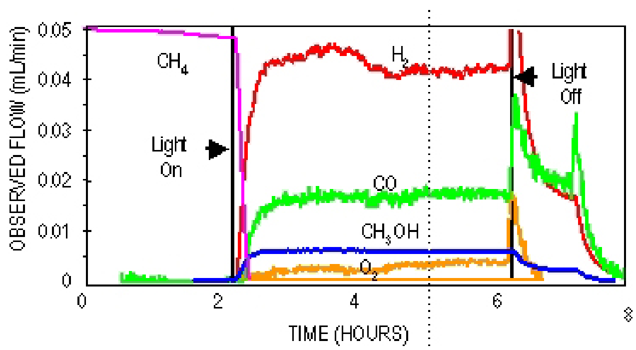
Economy:
Providing the public with affordable, ultraclean transportation fuels from a variety of domestic resources will help to sustain economic growth.



Vision 21 plant environment), and for small-scale purification of hydrogen (as in fuel cell-powered vehicles). For hydrogen to be used widely as a transportation fuel, improvements are needed in hydrogen storage. Hydrogen separation membrane development and its deployment in membrane reactor technology can offer potential advantages in hydrogen production and purification. An alternative approach is to use the appropriate starting fuels and novel reforming strategies.



There are a number of hydrogen storage technologies in various stages of maturity, but the use of advanced carbon materials offers new and exciting possibilities. Finally, the development of better methods for separating other materials in a refinery environment will be necessary to better control the chemical properties of advanced fuels.



Novel Synthetic Routes

Improved chemical routes are needed to convert natural gas and synthesis gas (produced from a variety of feedstocks by partial oxidation or gasification) to clean liquid fuels. Although some advances are possible in Fischer-Tropsch (F-T) processing, such technology has now matured to the point that further developments can be carried out by the industrial sector. The Focus Area will continue to investigate fundamental aspects of reactor hydrodynamics, catalysts, and advanced separation processes to achieve high product quality and yield of F-T fuels. In addition, the Focus Area will conduct fundamental research on other novel pathways for producing ultraclean fuels. Examples of such approaches include, but are not limited to, C-H bond activation, photochemical liberation of methane from gas hydrates, the development of biomimetic catalysts, and other novel routes to synthesize fuels, fuel additives, and related chemicals.