freedom CAR & vehicle technologies program

U.S. Department of Energy • Office of Energy Efficiency and Renewable Energy Oak Ridge National Laboratory

Fuels, Engines, and Emissions

Characterization of Transient Process Chemistry via Advanced Diagnostics

Background

High-efficiency advanced diesel engine technology is a leading near-term option for reducing petroleum consumption and oil imports in the United States. However, new regulations by the U.S. **Environmental Protection** Agency (EPA), to be phased in over the 2007-2009 model years, will require a 90% reduction in emissions of nitrogen oxides (NO_x) and particulate matter. Without development of improved engine-control strategies, new emission control systems and more advanced fuels, it is unlikely that diesel engines will achieve the new emissions standards.

Likely diesel solutions will combine advanced fuels, combustion regimes and catalysts. Catalysts for NO_x, sulfur and particulate control, are typically applied to open- or closed-cell honeycomb type structures which contain small channels millimeters wide and several inches long. In operation, these enginecatalyst systems exhibit temporally and spatially varying chemistry distributions throughout the system: e.g., enginegenerated hydrogen (H₂) pulses to effect catalyst performance. Measurement strategies capable of resolving such dynamic species distributions, including the intra-catalystchannel chemistry variations, are required to develop efficient diesel solutions to the emissions challenge.

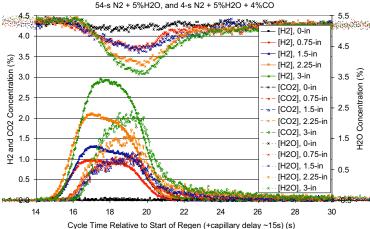
The Technology

The spatially resolved capillary-inlet mass spectrometer (SpaciMS) is a transportable instrument for quantifying the spatial and temporal distributions of emissions. The instrument was developed specifically for diesel catalysis research, but is applicable to other areas of research as well.

The SpaciMS uses a ^{0.5} minimally invasive capillary inlet system (200-micrometer outer diameter,10-milliliter per minute sampling rate) to transport time-varying species pools to a small mass spectrometer for analysis. A



Less dependence on foreign oil, and eventual transition to an emissions-free, petroleum-free vehicle



Pulsed Regen WGS Reaction @ 400C, SCONOx (K/Pt/Al2O3) Catalyst w/

The SpaciMS output shows the concentration of selected chemical species as a function of cycle time and location within the catalyst block. Fuels, Engines, and Emissions • Characterization of Transient Process Chemistry via Advanced Diagnostics

vehiele systems

multiport valve selects between up to twelve capillary sampling locations deployed throughout a test system (e.g., an enginecatalyst system). The minimally invasive nature of the sample capillaries allows for in situ analysis of full intracatalyst spatiotemporal species distributions.

With respect to understanding detailed catalyst chemistry this is a quantum leap from the previously available technology, which provided only catalyst-in and catalystout measurements, at much lower speeds. The broad species applicability of the SpaciMS allows analysis of a range of species critical to diesel catalysis, including NO_x, H₂, oxygen (O_2) , carbon dioxide (CO_2) , hydrocarbon fragments, sulfur dioxide, and hydrogen sulfide. The readily transportable nature of the SpaciMS has allowed for field application at industrial research laboratories.

Commercialization

The SpaciMS has been applied to make the first known measurements of H_2 generated via advanced in-cylinder diesel combustion strategies. Hydrogen plays a key role in catalyst performance and was also tracked throughout a catalyst system.

The SpaciMS has been used to monitor H_2 generated via the water-gas-shift reaction; the reaction of carbon monoxide (CO) and water (H_2O) over platinum to generate H_2 and CO₂. The figure on the previous page shows the intracatalyst dynamics of H_2 , CO₂ and H_2O associated with this reaction throughout a 3-inchlong catalyst. The phase and amplitude of the various dynamic species generations and depletion help to elucidate the detailed process chemistry.

ORNL has provided nine companies with information required to build and/or operate this system.

Benefits

- Broad species applicability
- Minimally invasive
- Quantifies intra-catalystchannel chemistry
- High temporal resolution
- Easily transportable

• Measures undiluted diesel engine exhaust

Where Can I Find More Information?

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A Strong Energy Portfolio for a Strong America

fuels & lubricants

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

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