Modeling Emissions Control Systems for Diesel Engines

Fuels, Engines, and Emissions

U.S. Department of Energy

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Oak Ridge National Laboratory

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Transportation

FOR THE 21ST CENTURY

Background

Under the direction of the U.S. Department of Energy (DOE) FreedomCAR and Vehicle Technologies Program, the Oak Ridge National Laboratory (ORNL) is coordinating research on new simulation tools for catalytic emissions control. Simulation tools are critical to enable engine and truck manufacturers to design emissions controls systems to meet future diesel engine emission goals.

The Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) is an R&D focus project of the Diesel Cross-Cut Team which is composed of representatives from U.S. diesel engine manufacturers, automotive companies, the DOE, the U.S. Army Tank Command, and the Environmental Protection Agency. The primary function of the Cross-Cut Team is to coordinate development efforts for advanced, low-emission, high-efficiency compression-ignition-direct-injection (CIDI) engines.

The overall objective of CLEERS is to promote development of improved computational tools for simulating realistic full-system performance of lean-burn engines and the associated emissions control systems. Other objectives include providing a consistent framework for sharing information and identifying R&D needs. Sponsored activities include a website and technical exchange workshops. In addition, the CLEERS committee is organizing a more targeted technical exchange mechanism referred to as Focus Groups. There will be three Focus Groups regarding each major emissions control technology (lean NO_x traps, diesel particulate filters, and urea selective catalyst reduction).

Success Story

The Technology

Since its beginning in 2001, five CLEERS workshops have been held focusing on the major thrust areas of diesel engine emissions control. The first workshop looked at overall system modeling; the second at NO_x adsorber technology; the third focused on diesel particulate filters (DPFs); the fourth and fifth on selective catalytic reduction (SCR) technologies both with and without urea/ammonia as reductants.

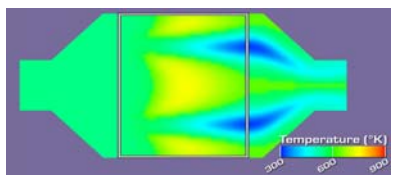
Each of these workshops identified key barriers to the success for the particular technology as well as R&D questions that needed to be addressed. For instance, the NO_x adsorber workshop identified the need for development of robust simulation tools for aging/sulfur poisoning; NO_x reduction catalysis, including the adsorption kinetics of NO on barium, cerium and sodium; and desulfation chemistry.

ORNL is developing adsorption and regeneration kinetics models for NO_x adsorbers. Prototype catalytic materials are exposed to flowing synthetic exhaust gas at different temperatures and gas compositions while both global and surface reaction rates are measured. These data are used to improve understanding of the chemistry and construct better predictions of LNT performance.

ORNL is making similar studies of selective catalytic reduction. The new models for these devices utilize recent discoveries that have significantly changed earlier understanding about how catalyst monoliths function.

Benefits

- Reduces cost and time needed to develop advanced diesel engine emissions controls.
- Diesel engine companies and truck manufacturers can apply the models to their specific systems.
- Will lead to faster implementation of new pollution control technologies as they become available.



This computational visualization shows temperature contours in a catalyst monolith during cold start. Catalyst cold start performance is critical to reducing emissions.

For more information on how ORNL is helping America remain Competitive in the 21st century, please contact:

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