CHEMKIN-PRO for Reciprocating Engine Applications

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Summary

This application note describes how CHEMKIN-PRO can be used to aid the design of piston engine applications such as passenger automotive, light- and heavy-duty trucks, locomotive, ship, and heavy-duty off-road vehicles.

Challenges Facing Piston Engine Designers

The automotive, truck, and marine piston engine market is facing new challenges to develop high-efficiency, fuel-flexible, alternative combustion strategies for low-emissions performance. Emissions requirements for automobiles and light-duty trucks have ratcheted down over 90% in the United States and Europe. Additionally, heavy-duty diesel engines are coming under new regulations requiring advanced after-treatment systems such as diesel particulate filters (DPF) and two- or three-way catalysts.

Simulation Strategy That Is Complementary to CFD

Piston engine designers have already adopted computer simulation of the engine cylinder with Computational Fluid Dynamics (CFD). While CFD tools are valuable in understanding engine-cylinder flow-field patterns, heat transfer and global chemistry, they often are not effective in handling the full chemistry details that are important for analyzing critical combustion issues. Most commercial CFD tools limit the number of species in the chemistry mechanism to 50 or fewer; however, full reaction mechanisms for realistic fuel models involve hundreds of species with thousands of reactions. Even without a 50-species limit, CFD with full chemistry would be fraught with solver instabilities or would take so long that it would not be effective in the engine-design workflow. Alternative methods are required where full detailed chemistry can be efficiently and effectively employed in engine design.

CHEMKIN-PRO Software has a number of capabilities that apply directly to the analysis of in-cylinder combustion and after-treatment performance simulation towards enhanced performance and low emissions. Here are some of the ways that CHEMKIN-PRO can be used in engine and after-treatment design:

- Calculate important combustion performance factors such as ignition delay and laminar flame speed.

- Conduct parametric variations on factors such as equivalence ratio, residence time, and fuel composition.
- Utilize the Multi-zone model to correctly predict emissions in HCCI engines.
- Simulate the catalytic performance of after-treatment systems on a component-by-component basis.
- Validate reduced reaction mechanisms for CFD simulations with the help of the Reaction Path Analyzer.
- Predict the relative dominance of chemical kinetics vs. turbulent mixing for a given set of conditions.
- Understand soot formation and oxidation mechanisms inside a piston engine.

About Reaction Design

Reaction Design helps transportation manufacturers and energy companies rapidly achieve their Clean Technology goals by automating the analysis of chemical processes via simulation and modeling solutions. Reaction Design is the exclusive developer and distributor of CHEMKIN and CHEMKIN-PRO, the *de facto* standards for modeling gas-phase and surface chemistry, providing engineers ultra-fast access to reliable answers that save time and money in the development process. Reaction Design also offers the CHEMKIN-CFD software module, which brings detailed kinetics modeling to other engineering applications, such as Computational Fluid Dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the production plant. Reaction Design serves more than 350 customers in the commercial, government and academic markets.

Reaction Design can be found online at www.reactiondesign.com.