Impact of Novel Fuel Components on the Performance of Three-Way Catalysts for Control of SI Engine Emissions

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Motivation
- DOE-funded Co-Optimization of Fuels and Engines Initiative aims to simultaneously develop high performance fuels and advanced high efficiency engines to reduce petroleum consumption
- To achieve commercialization, advanced engines running on novel fuels must still meet U.S. EPA emissions regulations
- Three-way catalysts (TWCs) are extremely effective at controlling emissions from SI engines when hot; cold start performance is critical for compliance, and will depend on fuel composition
- Evaluation of potential fuel components requires quantification of impact on TWC light-off behavior

Experimental Methods and Key Results
- Lambda ($\lambda$) sweep 0.999-0.995 with E10 surrogate fuel
  - $\lambda = \frac{\text{AFR}}{\text{AFR}_{\text{stoic.}}}$
- $\lambda = 0.999$ was selected for further light-off experiments

Impact of Fuel Light-off on other Regulated Pollutants
- Alcohols, straight-chain ketones, alkanes, esters and cycloalkanes have minimal effect on CO light-off
- Aromatic hydrocarbons, aromatic ethers, cyclic ketones, and alkenes have a significant impact on CO light-off → inhibition of CO oxidation until the HC reacts
- NOx $T_{50}$s comparable across different fuels because CO and H2 reduce a significant fraction of NOx
- NOx $T_{90}$s follow trends similar to the HC conversions: at $\lambda = 1$, high HC conversions are required to achieve high NOx conversions

Future Work
- Real-world fuels are complex multicomponent blends
- Key question: Can we predict the light-off behavior of a blend from the light-off profile of its pure components?
- "Simple" linear combination fails to accurately predict the blend light-off behavior
- Inclusion of thermal effects and chemical interactions on the catalyst surface may improve the predictions

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Synthetic Exhaust Flow Reactor Configuration
- Extensive range of liquid fuel components, including many oxygenates, makes this study unique
- Automated flow reactor controlled with LabVIEW
- Vapor delivery module used to introduce liquid fuel components
- FID, FTIR and MS used to analyze effluent from the reactor
- Catalyst aging and evaluation experiments conducted according to the U.S. DRIVE Low-Temperature Oxidation Catalyst Test Protocol*
  - Aged 50 h @ 800 C: neutral/rich/lean cycles
  - Reaction profile repeated 3x per fuel to ensure reproducibility of results

Selected Fuel Light-off Profiles over aged TWC
- Excellent reproducibility was achieved for all fuel components
- Light-off behavior depends on both functional groups and molecular structure (linear, branched, cyclic)
- Alcohols < linear ketone < long-chain alkane < ester, cycloalkanes < E10 surrogate < aromatic ethers, aromatic hydrocarbons < alkenes

*https://cleers.org/low-temperature-protocols/