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

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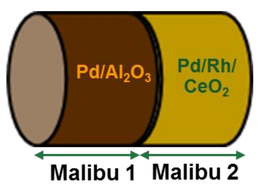
Acknowledgement: Funding provided by DOE Vehicle Technologies Office (Kevin Stork, Gurpreet Singh, Leo Breton, Mike Weismiller)

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

Catalyst

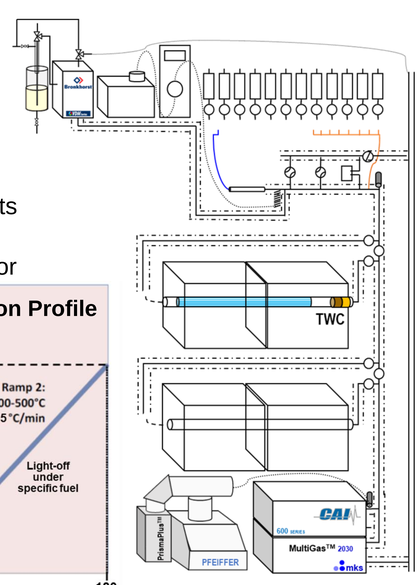


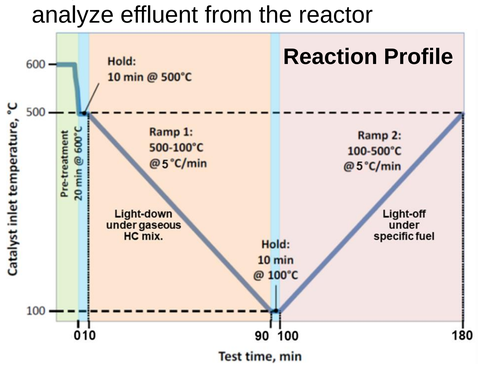
TWC	Pd (g/l)	Rh (g/l)
Malibu 1	7.3	0
Malibu 2	1.1	0.3

- Commercial three-way catalyst: MY2009 Chevy Malibu SULEV/PZEV close-coupled TWC
- Dual-zone: Pd-rich front end and Pd/Rh/ceria back end

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



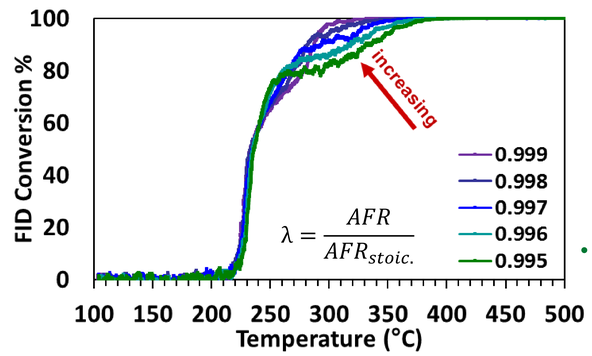


- Catalyst aging and evaluation experiments conducted according to the U.S. DRIVE Low-Temperature Oxidation Catalyst Test Protocol*
- Aged 50 h @ 800 C: neutral/rich/lean cycles
- Reaction profile repeated 3x per fuel to ensure reproducibility of results

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

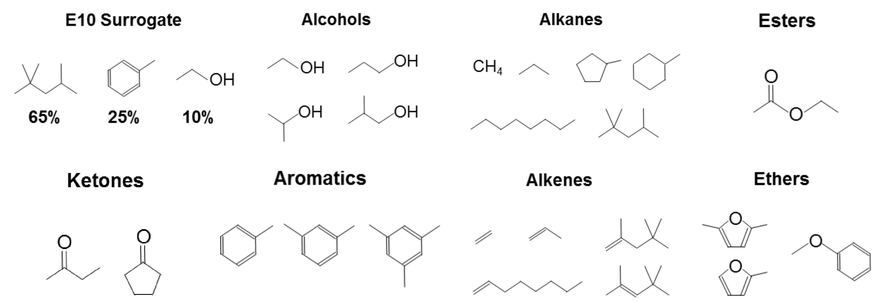
Experimental Methods and Key Results

Lambda (λ) sweep 0.999-0.995 with E10 surrogate fuel

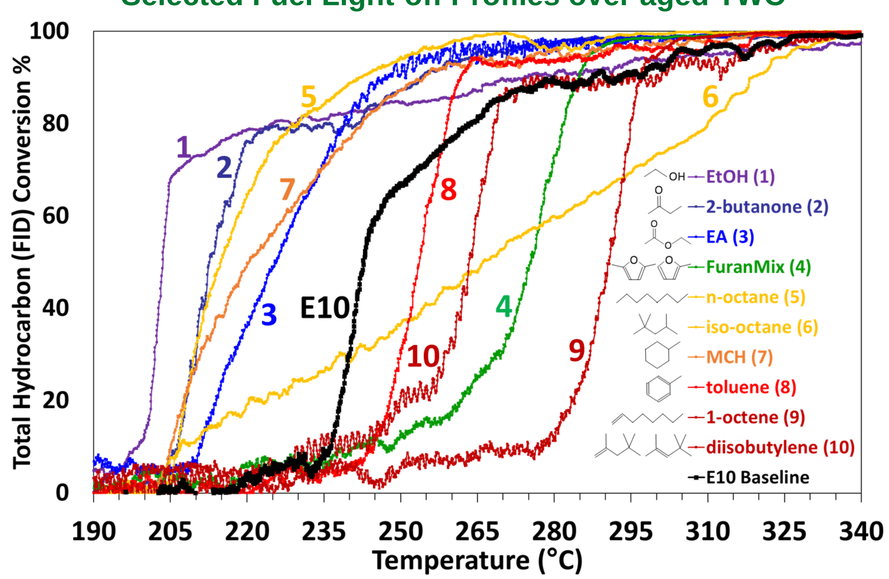


O_2 varied to adjust λ
13 % H_2O
13% CO_2
1670 ppm H_2
5000 ppm CO
1000 ppm NO
3000 ppm C_1 HC

- **λ = 0.999** was selected for further light-off experiments

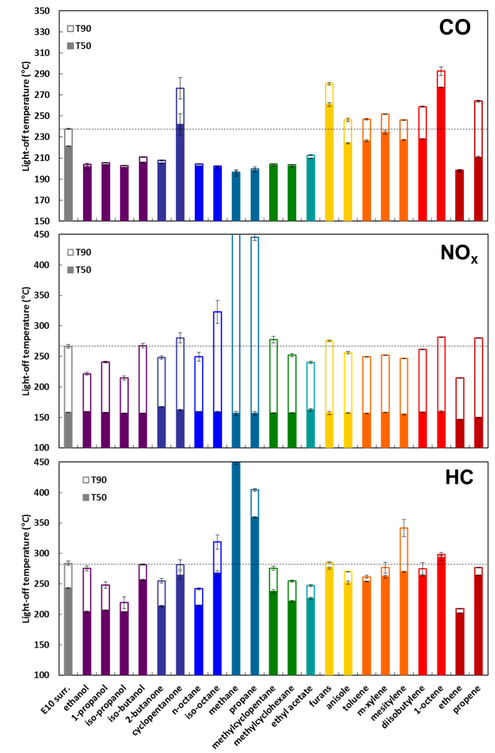


Selected Fuel Light-off Profiles over aged TWC



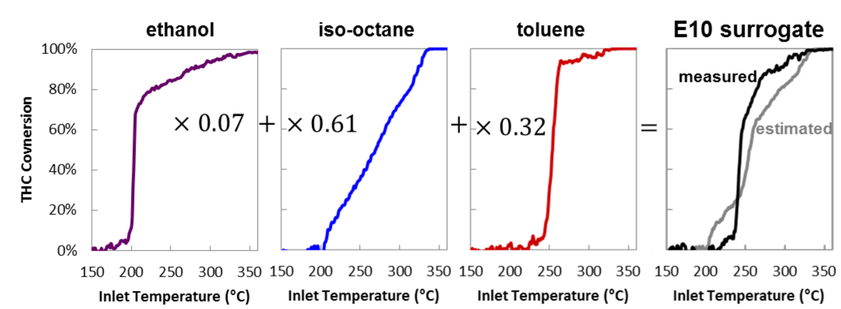
- Excellent reproducibility was achieved for all fuel components
- Light-off behavior depends on both functional groups and molecular structure (linear, branched, cyclic)
- Alcohols < linear ketone < long-chain alkane < ester, cycloalkanes **< E10 surrogate** < aromatic ethers, aromatic hydrocarbons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

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
- NO_xT_{50}s comparable across different fuels because CO and H_2 reduce a significant fraction of NO_x
- NO_xT_{90}s follow trends similar to the HC conversions: at λ = 1, high HC conversions are required to achieve high NO_x 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

Acknowledgements

We gratefully acknowledge valuable discussions with Bob McCormick, Dan Gaspar, and Jim Szybist and experimental support from Will Brookshear.