Motivation
- Meet the strict US emissions regulations by treating the high UHC and CO emissions from RCCI engine at low exhaust temperatures using a Diesel Oxidation Catalyst
- GT-Power is a system based modeling tool which is quite flexible and the effect of numerous variables on DOC performance can be observed
- Transient behavior cannot be interpolated from steady state because input variables change/fluctuate at a lot of different rates during transients

Objectives
1. Design a systematic procedure for the development of an aftertreatment DOC model for an RCCI engine in GT-Power
2. Steady State Operation: Calibrate and run various steady state cases and observe the effect of various inlet conditions and variables on DOC performance
3. Transient Operation: Observe the effect of various inlet conditions and variables on DOC performance and compare with steady state operation

Diesel Oxidation Catalyst and GT-Power Modeling

Catalytic reactions:

\[ \text{HC} + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2 \text{O} + \text{CO} \]

\[ \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2 \]

\[ \text{reaction rate} = \, 3.103 \, \times \, 10^{16} \, \exp \left( \frac{-159400}{T} \right) \, \text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1} \]

Surface catalyst loading = Dispersion factor * Molaric catalyst loading

Catalyst Specifications:
- Volume: 0.6 L
- Substrate dimension: 1096 mm x 1200 mm
- Substrate material: Metallic
- Case/wall thickness: 50/50 micron
- Loading/wt: 90 gTi-Pt

Data for Calibration:
- Inlet concentration of exhaust gases
- Inlet flow rate of exhaust gas
- Exhaust gas temperature
- Gas composition (mole fraction)
- Simulation time [sec]
- Time step size [sec]

GT-Power Model:
- Start with GT-Power "Basaltic and Sampara" model
- Warm-up behavior with air flow (O2 + N2)
- Geometrical and thermal inputs checked
- Calibrate POM active site density dispersion factor
- Match 50% light-off point of UHC and CO
- Calibrate active site density
- Match low temperature UHC/CO storage (if present)
- Modify activation energies and pre-exponential multipliers of oxidation reactions

RCCI Steady State Cases and Calibration

Steady State Analysis: Effect of Input Variables

Steady State Analysis: Effect of Precious Metals

Future Work
- Steady State Operation: Catalyst storage modeling at low loads, EGR modeling since EGR changes exhaust gas composition, Effect of other precious metals (Eg: Rh) and NOx modeling for some RCCI systems
- Transient Operation: Observe the effect of other input variables, Down speed and down load transient analysis and Other transient cases (Eg: Starting, simultaneous speed and load change etc.)
- Develop full scale integrated RCCI model (Aftertreatment model + Engine System model)