reaction DESIGN

CHEMKIN-PRO
Aftertreatment in Internal Combustion Engines

Engine aftertreatment is increasingly a focus for meeting emission requirements; three-way catalysts are a key part of engine aftertreatment systems. You can use CHEMKIN-PRO to simulate the catalytic reactions in engine aftertreatment systems to predict performance, such as percentage of reduction for NO_x, CO and unburned hydrocarbons (UHCs), and test catalytic reactor design and operating condition impacts. CHEMKIN-PRO offers reactor models supporting catalytic and aftertreatment simulations that are plug-and-play components with robust, proven kinetics capability.

Setting Up a Dynamic Engine Exhaust Aftertreatment Analysis

CHEMKIN-PRO provides the ability to track the dynamic levels of NO_x, CO, and UHC through catalytic surface reactions on a catalyst by reading in transient engine-out data to provide dynamic inlet conditions for an engine-exhaust aftertreatment simulation. A CHEMKIN-PRO Honeycomb Monolith catalytic reactor, combined with a catalytic mechanism, approximates a catalytic converter, designed to convert NO_x, CO, and unburned hydrocarbons (UHCs) through catalytic surface reactions on a platinum/rhodium catalyst.

Results

The simulation shows the growth and development of species through time, as illustrated in the figures below. Calculations for species conversions are shown in the plots that follow (Figure 1 to Figure 3). You can see in these figures that C_3H_6 (propene) and CO are converted more effectively than NO under these conditions. We can postulate that setting the initial conditions in the reactor to pure air, which determines the initial exit flow, is also responsible for the calculated molar conversion rate of 100% at t=0. The negative values for the calculated conversion rates for CO and NO at certain times result from the changing state of the catalyst surface: CO and NO can be formed on the surface, and can be "produced" when desorbed from the surface changes. Figure 3 shows inlet and exit gas temperatures as a function of time. Temperatures indicate that the gas heats up relative to the inlet gas due to exothermic surface reactions. This is consistent with the work reported by Chatterjee et al.[1]

[1]D. Chatterjee, O. Deutschmann and J. Warnatz, "Detailed Surface Reaction Mechanism in a Three-way Catalyst," *Faraday Discussions*, **119**:371-384 (2001).

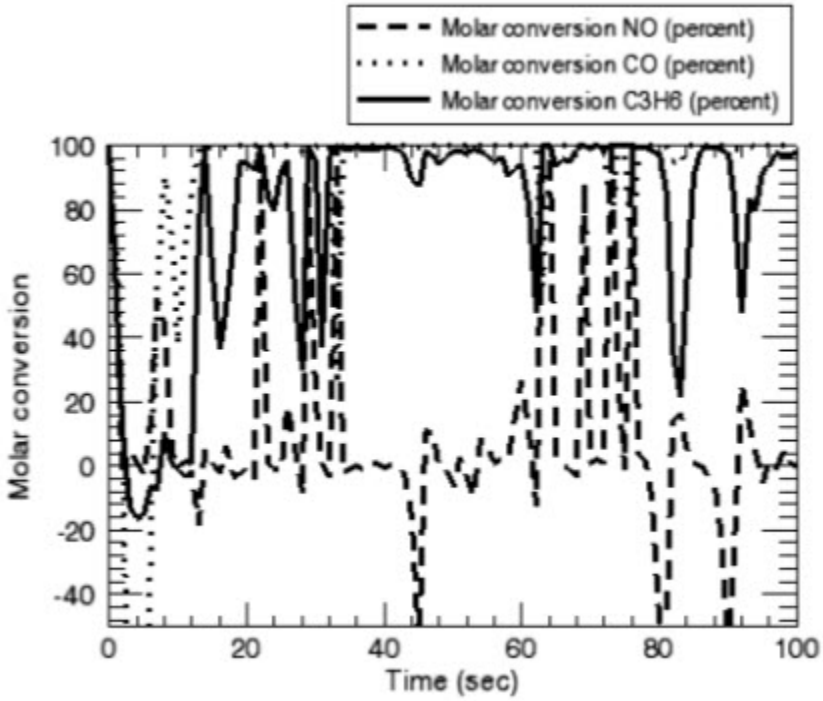

Figure 1. Molar Conversion Rates: NO converted least efficiently.

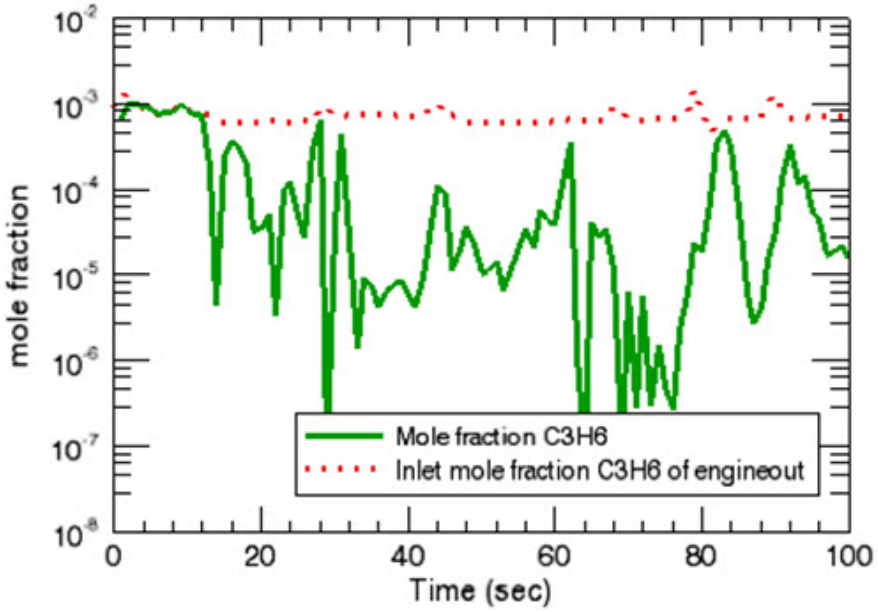

Figure 2. C_3H_6 (mole fraction): Dynamically converted.

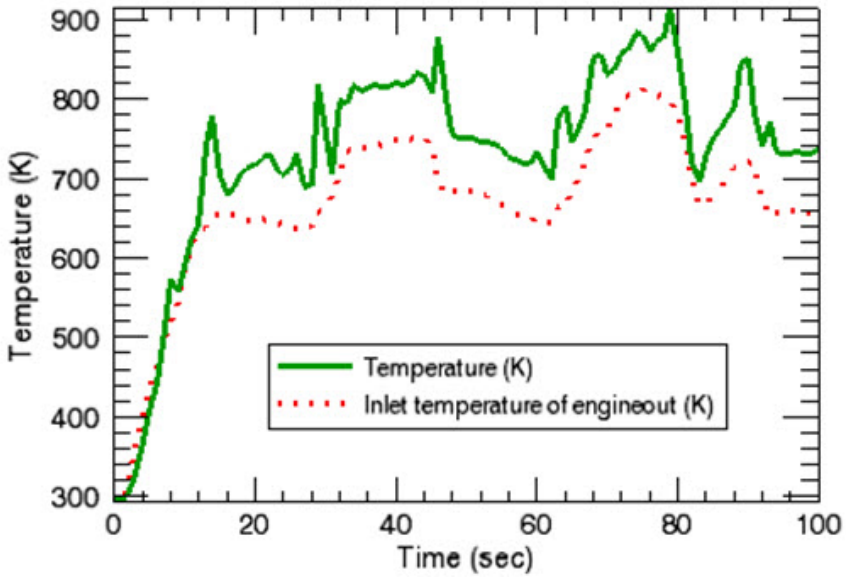

Figure 3. Temperatures of inlet and exit gases. Catalyst activity indicated at about 600K.