

Towards an Optimum Aftertreatment System Architecture

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ABSTRACT

Aftertreatment system design involves multiple tradeoffs between engine performance, fuel economy, regulatory emission levels, packaging, and cost. Selection of the best design solution (or “architecture”) is often based on an assumption that inherent catalyst activity is unaffected by location within the system. However, this study acknowledges that catalyst activity can be significantly impacted by location in the system as a result of varying thermal exposure, and this in turn can impact the selection of an optimum system architecture. Vehicle experiments with catalysts aged over a range of mild to moderate to severe thermal conditions that accurately reflect select locations on a vehicle were conducted on a chassis dynamometer. The vehicle test data indicated CO and NOx could be minimized with a catalyst placed in an intermediate location. The vehicle data was also used to calibrate a single channel monolith catalyst model (via adjustment of kinetic parameters) to match each of the different aged conditions. The calibrated model forecasted an optimum configuration with a close-coupled front brick and an underbody rear brick. Subsequent vehicle experiments confirmed the model predictions. The modeling approach can be extended to investigate an optimum architecture for other applications as well.

CITATION: Katare, S., Hubbard, C., and Son, S., "Towards an Optimum Aftertreatment System Architecture," *SAE Int. J. Engines* 8(1):2015, doi:10.4271/2015-26-0104.

INTRODUCTION AND BACKGROUND

Government regulations have driven down allowable exhaust emission levels significantly across the world, and catalysts play a critical role in our ability to achieve these levels as well as contribute a significant part of the engine and powertrain cost. Location of the catalyst within the exhaust system is a key factor that determines how well the catalyst performs. Key factors governing this location are the catalyst inlet temperature, packaging constraints, catalyst washcoat light-off temperature, engine emission levels and the required tailpipe levels.

If catalyst performance did not degrade with exposure to high temperature, a catalyst placed closest to the engine would warm-up during the cold start and light-off fastest to result in the lowest emissions. However, a catalyst that is placed closest to the engine also experiences the highest temperatures over its lifetime which can lead to the most severe deactivation. In contrast, a catalyst that is located farther from the engine exhaust manifold will experience less severe thermal damage, but its overall performance may suffer due to poor catalyst light-off. An optimum catalyst location is the result of the best trade-off between catalyst durability and ease of light-off. Placing the catalyst closest to the engine may not always be the most optimum location for controlling emissions. An intermediate location that is close enough to the engine to afford a reasonable light-off potential with minimal PGM and yet be far enough away to result in only moderate damage over the lifetime of the catalyst may yield optimum performance.

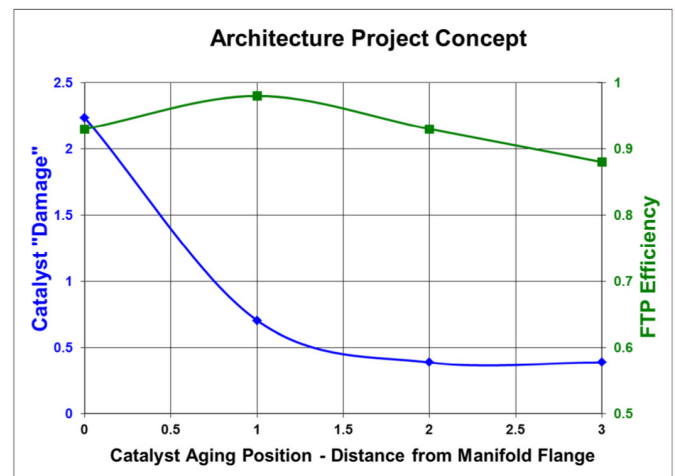


Figure 1. Graphical depiction of the base concept of this study that relates catalyst location to deactivation level or “damage” and FTP emission cycle performance.

Figure 1 graphically depicts the base concept of this study. A catalyst that is located closest to the manifold flange experiences the highest temperatures which in turn results in the most severe damage. FTP efficiency is a combination of how fast the catalyst heats up and lights off, and as well as how much damage the catalyst has sustained. A catalyst placed farthest away from the engine may experience the least amount of damage, but also experience the slowest light-off and poorest performance. When the catalyst is placed closest to the engine it experiences the highest inlet

temperature and possibly fastest light-off; however, due to sustained exposure to higher temperatures the catalyst in this location is the most severely damaged. The trade-off between thermal damage and light-off performance results in an intermediate optimum location, as shown in the figure, where the FTP efficiency peaks. The goal of this aftertreatment architecture project is to develop an understanding of this intermediate location for a specific application so as to maximize the aftertreatment performance, and then apply this understanding to other applications. Finding the optimum location can help reduce exhaust backpressure, lower cost through lower precious metal loadings, provide alternative packaging options, and perhaps improve flow uniformity by providing more space for entrance/exit cones.

Specific objectives of this study are (1) to generate vehicle data to define the relationship between emission performance and catalyst aging position for a specific powertrain, (2) to calibrate a mathematical model of TWC performance ("SimCat") to extract the relationship between catalyst activity and catalyst damage, (3) to exercise the calibrated model to determine optimum configuration for the powertrain evaluated, and (4) to establish guidelines to extend this modeling application to other powertrains and catalyst washcoat combinations.

The rest of this paper is organized as follows. [Section 2](#) deals with the literature study with emphasis on catalyst location studies. Vehicle data obtained as part of this study and its analyses are reported in [Section 3](#). The model calibration and results of using the calibrated model in projecting optimum aftertreatment configuration is explained in [Section 4](#). The final Section summarizes the report and offers general conclusions and possible extensions of this work.

LITERATURE STUDY

A catalyst is a substance that increases the rate of a reaction without modifying the overall standard Gibbs energy change in the reaction. The conversion in a catalytic reaction often decreases with time. This phenomenon is called catalyst deactivation. Causes of deactivation typically fall under three categories: chemical (poisoning, vapor compound formation accompanied by transport and vapor-solid and/or solid-solid reactions), mechanical (fouling, attrition and crushing) and thermal [1].

Catalyst deactivation can result from changes in the structure or in the texture of the catalyst. Such changes are usually irreversible and the catalyst cannot be regenerated. Due to sustained exposure of the catalyst to high temperatures over time the distributed active sites on the catalyst surface agglomerate either due to atomic or crystallite migration resulting in the loss of active surface area for reaction [2]. This thermally activated physical process that results in the loss of active surface via structural modification of the catalyst is known as sintering and it forms the basis of one of the key irreversible catalyst deactivation mechanisms. Exposure to poisons such as carbon, phosphorus and sulfur can reduce the conversion of catalytic processes; however, periodic thermal treatment of the catalysts may reverse such deactivation processes.

Studies on catalyst deactivation are critical to understanding how catalyst activity degrades over a period of time [3]. This helps design more durable catalysts that can sustain longer exposure to higher temperatures common over the useful period of an automobile catalyst. Significant time and resources have been spent by the OEMs, catalyst suppliers and universities in understanding accelerated ageing techniques to study the degradation of catalyst efficiency with exposure to thermal cycles and poisons in the fuel over a period of time. Attempts at correlating thermal "damage" of the catalyst to catalyst activity parameters have predicted an exponential Arrhenius relationship between activity loss and catalyst "damage". Such detailed empirical studies have been very useful as rules of thumb in generating target damage values for a given threshold emission performance and also to predict vehicle tailpipe emissions for changes in full useful life catalyst ageing cycles.

The mechanism of thermally induced catalyst activity loss on various criteria pollutants may be significantly different. CO oxidation and NO_x reduction are highly dependent on oxygen storage capacity (OSC) and hence loss of OSC due to thermal damage significantly reduces the conversion efficiency of CO and NO_x. In contrast, HC oxidation is a mostly PGM based light-off controlled process and so significant exposure of catalysts to high temperatures may not reduce the catalyst HC efficiency as long as the catalyst PGM content is maintained. Thus moving the catalyst closer to the engine significantly reduces HC emissions as compared to other emissions.

VEHICLE DATA

A Ford mid-sized petrol vehicle was fitted with a prototype aftertreatment system at three different locations along the exhaust path. At each catalyst location, the catalyst effective temperature, T_{eff} , was measured on the SRC (Standard Road Cycle) on an engine dynamometer. From this data the accelerated ageing time/temperature were determined by proprietary Ford's EPA approved Arrhenius analytical model. In this Arrhenius model, the exponentially weighted average catalyst midbed temperature that the catalyst experiences over an SRC cycle, either on the road or on an engine dynamometer bench is related to the catalyst midbed temperature from the Ford 4-Mode engine bench cycle by equating the tailpipe emission values.

Time duration required to age a catalyst in an accelerated fashion at this temperature in an engine dynamometer bench in order to simulate the vehicle-aged catalyst over its full useful life is analytically calculated.

In the current study the "Close-Coupled" (CC) location closest to the engine was at a distance of a few inches from the engine exhaust manifold flange. The catalyst at this location was aged under the most stringent accelerated Ford ageing cycle regimen at the highest temperature and the longest duration. The second location chosen in this study was "Underbody" (UB) wherein the catalyst was located downstream if the CC location. The "Muffler" location with the most lenient ageing regime of located the catalyst the farthest from the engine manifold flange. Each of the accelerated ageing criteria was chosen based on the time temperature cycle that the catalyst would experience over its full useful life when placed at the respective locations. The key idea was that the catalysts located at each of these

three locations would experience different temperatures over different periods of time and hence would age differently and would have their activity degraded at different rates.

The catalyst system on the vehicle chosen for this study was in the form of two bricks separated by a one inch gap. The first brick was smaller in volume, with a higher cell density, smaller wall thickness, and higher PGM loading so as to enable faster light-off. The catalyst washcoat chosen in this study was a production version from a Ford supplier.

The vehicle was tested in a chassis dynamometer with the capability to record sec $\times$ sec modal emission information and accumulated regulation based bag data. Emissions were recorded at the feedgas and tailpipe locations. Temperatures at multiple locations were recorded using a 1/8" thermocouple which was then used to obtain the true gas temperature with the help of a proprietary model that accounts for the thermocouple size and other physical characteristics. Figure 2 shows the thermocouple corrected catalyst inlet temperatures experienced by the catalysts at each of the CC, UB and Muffler locations over the first bag of an FTP test. It is interesting to note that the catalyst inlet temperature of the CC catalyst was 125C to 150C higher than that at the UB location.

The quality of the emission data obtained from the chassis dynamometer as measured by the match between bag 1 data and accumulated modal data over the first 505 seconds of the FTP test with the CC aged catalyst located at the CC, UB and Muffler locations is shown in Figure 3. The match between the bag and modal data suggests that the data is of very good quality. Figure 4 shows a comparatively larger scatter between the bag and modal data for the tests with the catalyst aged at the UB location; however, the match is still reasonably good for the purpose of calibrating the model to data. Match between bag data and modal data for the Muffler aged catalyst is shown in Figure 5. Though the NOx modal data seems to be lower compared to the corresponding bag data, the overall quality of the data is still fairly good for the purposes of this study. Data in Figures 3, 4, 5 have been normalized by the maximum of the CO bag values from each of the three test locations.

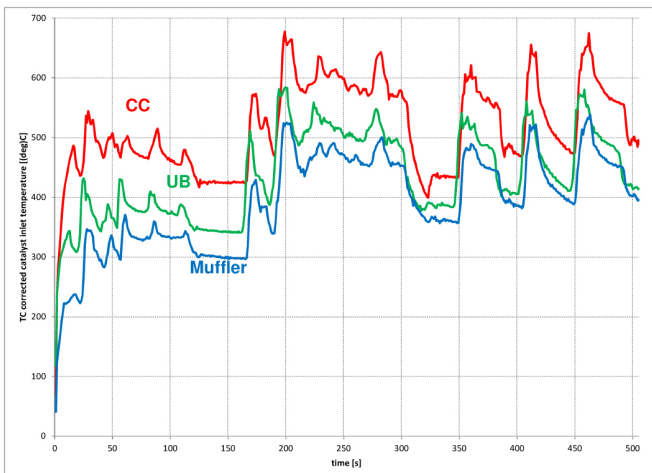


Figure 2. Thermocouple corrected catalyst inlet temperatures at the CC, UB and Muffler locations.

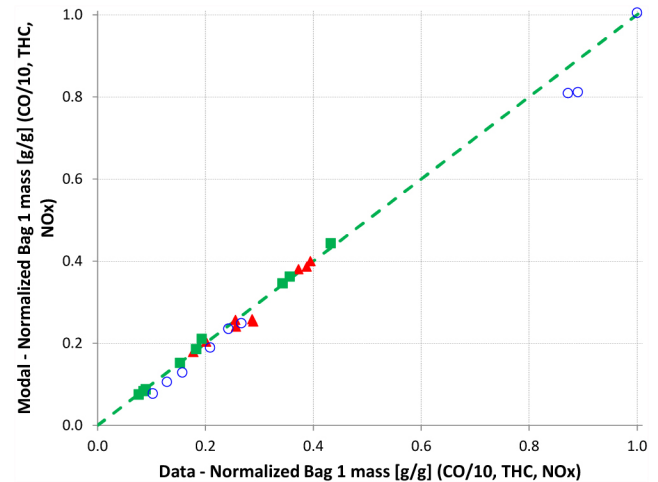


Figure 3. Normalized vehicle data with the CC aged catalyst tested at the CC, UB and Muffler locations. CO is represented by triangles, THC by squares and NO by circles.

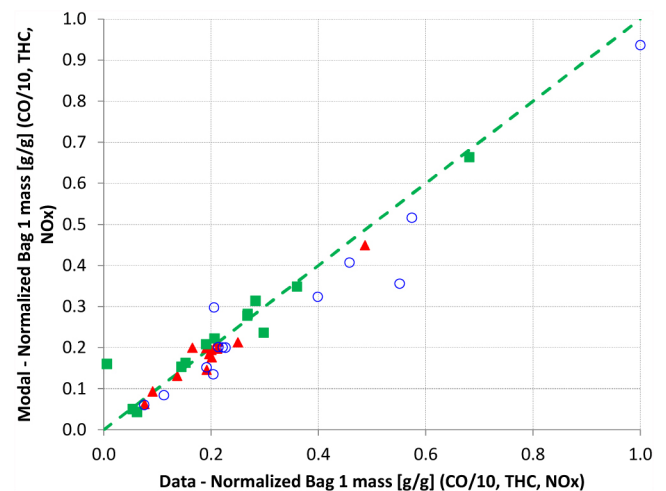


Figure 4. Normalized vehicle data with the UB aged catalyst tested at the CC, UB and Muffler locations. CO is represented by triangles, THC by squares and NO by circles.

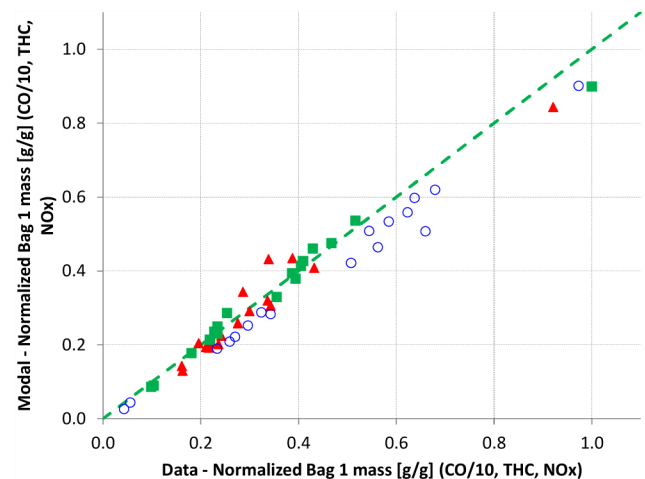


Figure 5. Normalized vehicle data with the Muffler aged catalyst tested at the CC, UB and Muffler locations. CO is represented by triangles, THC by squares and NO by circles.