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A New Semi-Empirical Temperature Model for the Three Way Catalytic Converter

Stefano Sabatini*, Irfan Kil**, Joseph Dekar ***, Travis Hamilton ***, Jeff Wuttke ***, Michael A Smith ***, Mark A Hoffman*, Simona Onori*,**

* Department of Automotive Engineering- Clemson University, Clemson, SC 29607 USA
** Department of Electrical and Computer Engineering - Clemson University, Clemson, SC 29634 USA
e-mail: (ssabati, ikil, mhoffm4, sonori@clemson.edu)
*** FCA US LLC - Auburn Hills, MI 48326 USA
e-mail: (joseph.dekar, travis.hamilton, jeff.wuttke, michael.a.smith@fcagroup.com)

Abstract: This paper proposes a semi-empirical model to predict the temperature of the three-way catalytic converter. The model is derived from the partial differential equations describing the energy balance in the catalyst and it is simplified by lumping the heat produced by the exothermic reactions occurring in the catalyst into a single parameter. This simplification allows the model to be run real time in production vehicles, since no information about the concentration of the chemical species in the exhaust gas is requested as input to the model. The parameters are identified using a particle swarm optimization algorithm. It is shown that the model accurately predicts the system behavior.

1. INTRODUCTION

Future tightening of emissions standards and the 54.5 mpg fleet wide average fuel efficiency target on production vehicles by 2025 have spurred great interest from automotive companies toward the modeling, control and optimization of engine and aftertreatment systems (EPA, 2011). The Three Way Catalyst (TWC) has been extensively used to reduce oxides of nitrogen (NOx), and to oxidize hydrocarbons (HC) and carbon monoxide (CO) in current production vehicles.

The conversion efficiency of the TWC is highly dependent on temperature, as shown in Figure 1. The "light-off temperature" is defined as the temperature at which the desired reduction efficiency reaches 50% (Brandt et al., 2000). The time it takes the catalyst temperature to reach light-off temperature should be minimized for improved TWC functionality. Also, knowing and monitoring the catalyst temperature is crucial to: 1) protect the TWC from excessive temperatures leading to premature TWC failure and 2) estimate the temperature dependent oxygen storage component (OSC) of the catalyst. Models can be used to estimate the catalyst temperature in that they are a more cost effective alternative to temperature sensors.

A significant amount of research has been dedicated to modeling the TWC. Two modeling approaches are predominant in literature: physics-based modeling and empirical modeling. Physics-based models of the TWC are developed in Auckenthaler (2005), Montenegro and Onorati (2009), Kang et al. (2014),Kumar et al. (2012) and Depcik and Assanis (2005). In those works, converter operation was described using energy and mass balance equations with the purpose of predicting conversion of undesired engine emission species within the catalyst. Since the performance of the catalyst strongly depends on temperature, these models estimate catalyst temperature by solving a system of partial differential equations describing the energy balance coupled with a detailed chemical kinetics model. The estimation of the kinetic parameters makes the identification of these models quite challenging. In addition, due to their computational complexity, these models are not suitable for real time catalyst temperature estimation and OSC control.

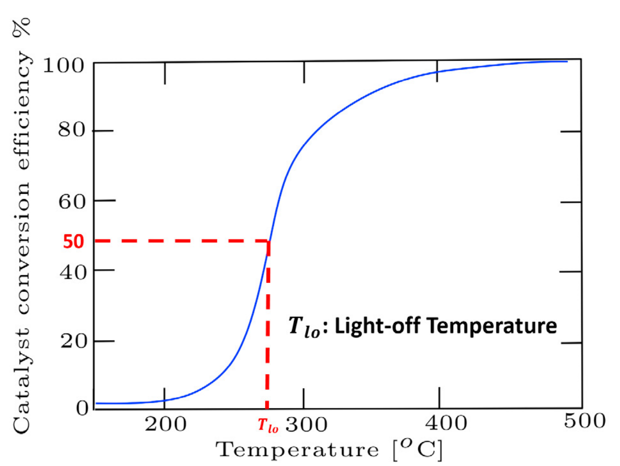

Fig. 1. The effect of temperature on a TWC conversion efficiency (jointly for CO, HC and NO_x) (reproduced from Bresch-Pietri et al. (2013)).

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Empirical models, like those developed by Shafai et al. (1996), Ammann et al. (2000), Brandt et al. (2000), Roduner et al. (1997), Cioffi et al. (2001) and Tomforde et al. (2013) are more computationally suitable for real-time catalyst monitoring and control. The objective of these models is to estimate the oxygen storage dynamic, which highly influences the exhaust gas emissions during transients. The models presented in Brandt et al. (2000) and Cioffi et al. (2001) also include catalyst temperature estimation. In Brandt et al. (2000) the temperature estimation is used as an input to a static catalyst conversion efficiency map in order to predict CO, NO and HC emissions. In Cioffi et al. (2001), the adsorption rate of an empirical oxygen storage model depends on temperature estimation. In both cases, the models consist of a first order differential equation whose parameters are empirically identified. Because of their simplicity, these models lack accuracy and are not reliable over wide ranging operating conditions, especially during the warm-up phase.

In Bresch-Pietri et al. (2013) a control-oriented TWC temperature model is obtained by simplifying the partial differential equations describing the energy balance into a time-varying input delay model. In that work TWC inlet concentrations of CO, NO and HC are model inputs for characterization of reaction heat. While complex models can approximate reaction heat through species estimation from lambda, actual species measurement are not available in production vehicles. Models this complex are not directly suitable for real time operation.

This paper presents a new semi-empirical temperature model suitable for real time vehicle operation. The model, suitable for control purposes, simulates thermal transients inside the catalyst. The heat produced by the chemical reactions is lumped into a single term so that the species concentrations are not necessary inputs. Experimental results, obtained under real driving conditions, demonstrate the accuracy of the model.

This paper is organized as follows: Section 2 provides information about the TWC system. The temperature model development is described in Section 3. In Section 4 the experimental setup used for model identification and validation is presented. Section 5 focuses on the parameter identification procedure and, in Section 6, the experimental results are presented and discussed.

2. TWC SYSTEM

Modern TWC converters are capable of conversion efficiencies approaching 100% when the catalyst is properly heated and the air fuel ratio is controlled in a narrow band around the stoichiometric value. However, conversion efficiency describes only the steady state behavior of the TWC while tailpipe emissions are highly affected by transient variations of the pre-catalyst air fuel ratio. The dynamic behavior of the TWC is dominated by its ability to store and release oxygen. For this reason, a considerable number of empirical oxygen storage models have been developed (Shafai et al., 1996; Ammann et al., 2000; Brandt et al., 2000; Roduner et al., 1997; Tomforde et al., 2013). Most oxygen storage models neglect the dependence of oxygen storage dynamics on catalyst temperature. In fact, catalyst temperature affects the reaction rates occurring in the TWC and consequently the oxygen adsorption and release rates.

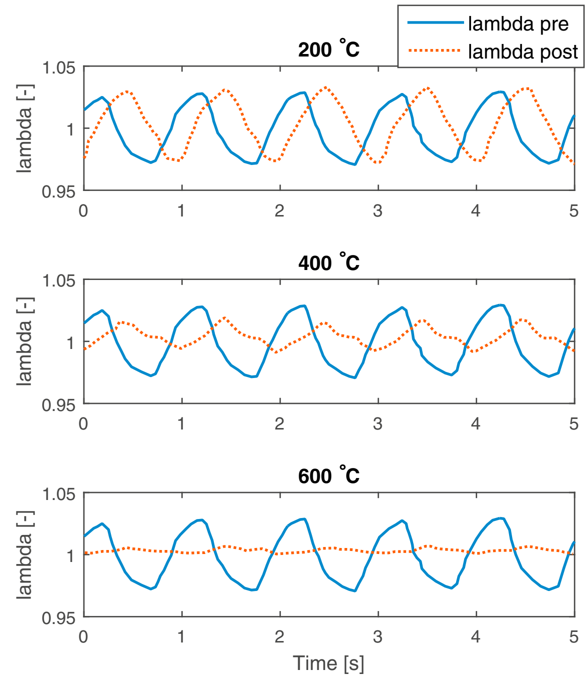

Fig. 2. Effect of temperature on the oxygen storage dynamics (reproduced from Brinkmeier (2006)).

In Brinkmeier (2006), the temperature dependence of the oxygen storage dynamics is proven empirically by the results shown in figure 2. In this experiment an oscillating air-fuel ratio profile is imposed upstream of the catalyst and the air fuel ratio response downstream the catalyst is evaluated for different catalyst temperatures. The higher the temperature, the more the oxygen storage influences the post catalyst lambda response. At low temperatures, besides the transport delay, the post catalyst lambda replicates the pre catalyst lambda. At $600°C$ the air fuel ratio oscillations are completely absent in the post TWC lambda due to the ability of the catalyst to store and release oxygen. It is indeed important to estimate the catalyst temperature and include its effect in the OSC modeling.

The proposed TWC control oriented model can be represented by the structure of figure 3. The catalyst thermal model is designed as a function of exhaust gas temperature (T_{exh})and exhaust mass flow rate ($\dot{m}_{exh}$) measured upstream of the catalyst. Inputs to the oxygen storage model are: 1) pre-catalyst lambda (measured), λ_{pre}, 2) exhaust mass flow (measured), $\dot{m}_{exh}$ and 3) catalyst temperature (estimated by the proposed thermal model) $\hat{T}_{cat}$. The model inputs λ_{pre}, $\dot{m}_{exh}$ and T_{exh} can be either measured by commercially available sensors (oxygen sensors, air mass flow meters, thermocouples) or calculated by the ECU. The overall outputs of the TWC are: oxygen storage (state estimated), $\hat{\Phi}$, catalyst temperature (estimated), $\hat{T}_{cat}$, and post-catalyst lambda (measured), $\hat{\lambda}_{post}$.
This paper focuses on the development, identification and validation of the catalyst thermal model.