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

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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

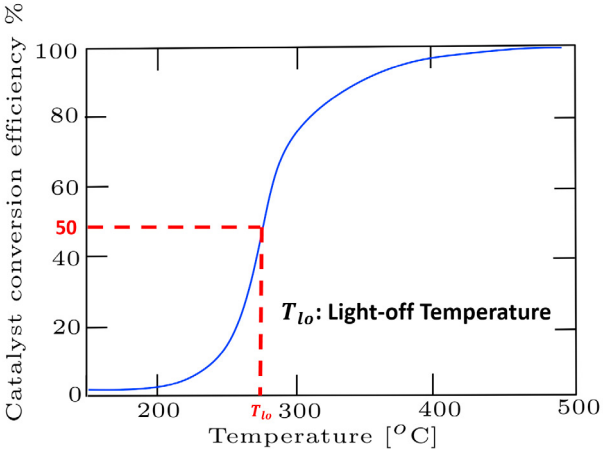

Fig. 1. The effect of temperature on a TWC conversion efficiency (jointly for CO, HC and NO_x) (reproduced from Bresch-Pietri et al. (2013)).

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.

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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.

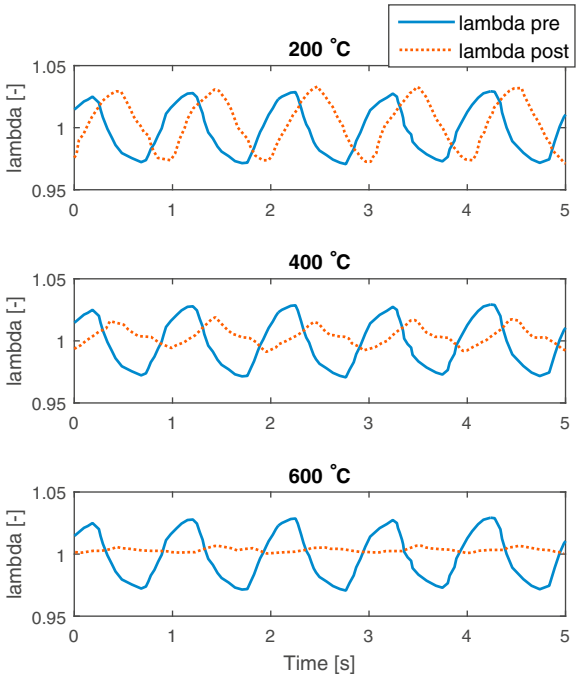

Fig. 2. Effect of temperature on the oxygen storage dynamics (reproduced from Brinkmeier (2006)).

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.

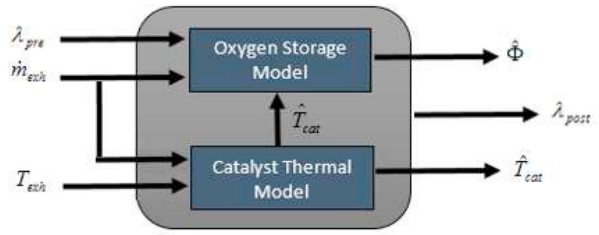

Fig. 3. Proposed structure of TWC.

3. TWC TEMPERATURE MODEL

Using a one dimensional approach, the TWC can be described as a single channel consisting of a gas phase and a solid phase. The gas phase represents the exhaust gas flowing into the converter and the solid phase represents the catalyst washcoat and substrate. The temperature dynamics of the TWC can be described by performing the energy balance on the gas phase and the energy balance on the solid phase.

The energy balance of the gas phase can be written as:

$$\rho_g \epsilon c_{p_g} \frac{\partial T_g}{\partial t} = \epsilon \lambda g \frac{\partial^2 T_g}{\partial z^2} - \frac{\dot{m}_{exh}}{A_{cs}} c_{p_g} \frac{\partial T_g}{\partial z} + h A_{geo}(T_{cat} - T_g) \tag{1}$$

where the first term on the right hand side accounts for the heat conduction and the second term for the convective heat transport in the axial direction. The last term describes the heat exchange between the gas and the solid phase. In a similar way the energy balance for the solid phase is performed resulting as:

$$\begin{aligned} \rho_s(1-\epsilon)c_s \frac{\partial T_{cat}}{\partial t} &= (1-\epsilon)\lambda s \frac{\partial^2 T_{cat}}{\partial z^2} - h A_{geo}(T_{cat} - T_g) \\ &+ A_{cat} \sum_j (-\Delta H_j R_j) - \frac{A_{out}}{V_{cat}} h_{out}(T_{cat} - T_{amb}) \end{aligned} \tag{2}$$

It is assumed that no transport phenomena are present in the solid phase. The term $A_{cat} \sum_j (-\Delta H_j R_j)$ accounts for the heat produced by the exothermic reactions occurring in the catalyst where R_j stands for the net reaction rate of each single chemical reaction occurring in the converter. In order to estimate the reactions rates, an accurate kinetic model should be developed and another system of PDEs should be added to the energy balance to account for the chemical species mass balance. Developing a kinetic model requires an extensive experimental campaign and a time consuming parameter calibration, in addition the model complexity would increase dramatically. Moreover, accounting for reaction kinetics, would require measurements of the concentrations of chemical species in the exhaust gas at the inlet of the converter.

For these reasons, simplifications will be made to the model in order to obtain a model suitable for real time applications.

Since gas phase conduction has a minor influence on catalyst temperature it can be neglected (Depcik and Assanis, 2005). In addition, given that the dynamics of the gas phase are much faster than the dynamics of the catalyst temperature, the storage term in equation (1) can be neglected, leaving T_g at steady state. In Montenegro and Onorati (2009) the authors showed the influence of each term in equation 2 on the catalyst temperature. From that study it is clear that the heat exchanged with the gas and the heat coming from the exothermic reactions are the dominant factors during normal catalyst operation. Conduction along the substrate is less important due to the low conductivity of the substrate material (cordierite) and therefore can be neglected. In TWC converters with a metallic substrate the conduction effect may not be negligible. The heat lost to the ambient becomes relevant at high temperature and is kept in the energy balance. As already mentioned, the development of a kinetic model is not suitable for control purposes. Therefore the heat produced by the chemical reactions is lumped into a single term $\dot{Q}_{reac}$. This term is related to the catalyst efficiency and dominates the energy balance after light-off while it is close to zero for temperatures below the catalyst light-off. Furthermore $\dot{Q}_{reac}$ is considered proportional to the exhaust mass flow rate $\dot{m}_{exh}$ and no dependence from the inlet species concentration is considered.

$$\dot{Q}_{reac} = K_{reac} \dot{m}_{exh} \eta(T_{cat}) \tag{3}$$

This assumption is accurate as long as the catalyst operates around stoichiometric conditions where the majority of the hydrocarbons and carbon-monoxide are reduced by the incoming oxygen. This is assured by today's air-fuel ratio controls that have the goal to keep the lambda upstream of the catalyst very close to 1, allowing only fast deviations from the stoichiometric value. If the catalyst is operated for a long period in severe lean or severe rich conditions, the modeling of the heat produced by the chemical reactions is not expected to be accurate. The TWC efficiency has been chosen to be an hyperbolic function of the catalyst temperature trying to reproduce the s-shaped efficiency behavior presented in literature (e.g. Kang et al. (2014)):

$$\eta(T_{cat}) = 0.5 tanh(s(T_{cat} - T_{light-off})) + 0.5 \tag{4}$$

where s is a parameter describing the slope of the efficiency curve while $T_{light-off}$ represents the catalyst light off temperature (figure 4). In conclusion the PDEs 1 and 2 are simplified as:

$$\frac{\dot{m}_{exh}}{A_{cs}} c_{p_g} \frac{\partial T_g}{\partial z} = h A_{geo}(T_{cat} - T_g) \tag{5}$$

$$\begin{aligned} \rho_s(1-\epsilon)c_s \frac{\partial T_{cat}}{\partial t} &= -h A_{geo}(T_{cat} - T_g) \\ &+ \dot{Q}_{reac} - \frac{4}{D_{cat}} h_{out}(T_{cat} - T_{amb}) \end{aligned} \tag{6}$$

To enable simulation, PDEs 5 and 6 are discretized in 100 computational nodes using an upwind finite difference

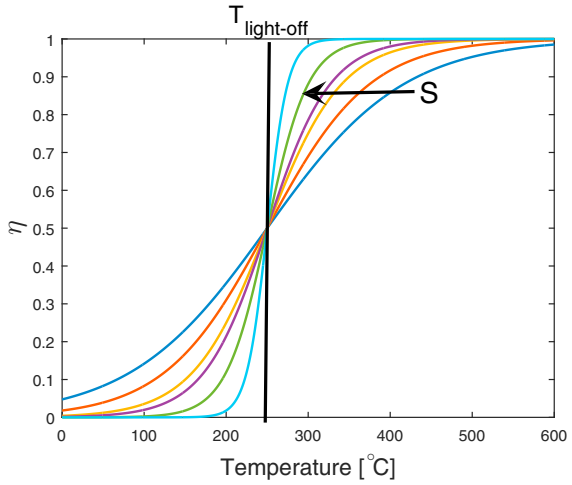

Fig. 4. Model of the TWC efficiency.

scheme. Since the real time capability of the model has to be preserved, the explicit Euler forward method is employed to integrate the equations because of its low computational demand. A sensitivity study with respect to the number of computational nodes is discussed in section 7. The boundary and initial conditions are:

$$\begin{aligned} T_g(t)\Big|_{x=0} &= T_{exh}(t) \\ T_{cat}(x)\Big|_{t=0} &= T_{cat_0}(x) \end{aligned} \tag{7}$$

4. EXPERIMENTAL SETUP

All the experiments for model identification and validation were performed on a FCA production vehicle in a chassis dyno test-cell. The catalyst was instrumented with one thermocouple at the inlet of the TWC measuring the exhaust gas temperature and one thermocouple located inside the catalyst brick to measure the substrate catalyst temperature. This second thermocouple is instrumented at the brick mid-length location as shown in figure 5. Even though no lambda measurements are needed as input to the proposed thermal model, a wide band lambda sensor placed at the TWC inlet is used for the validation and discussion in section 6.

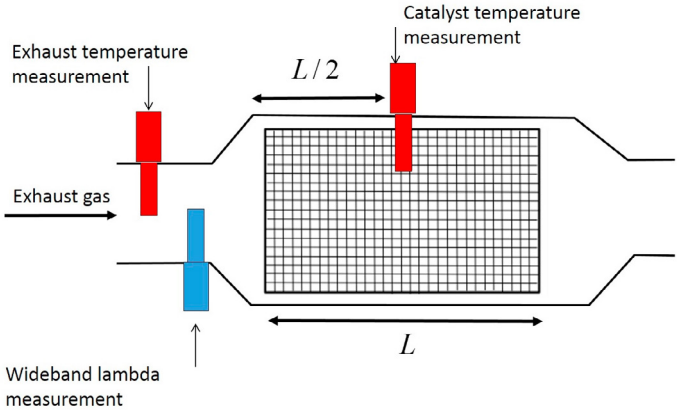

Fig. 5. Scheme of the sensors configuration

5. PARAMETERS IDENTIFICATION

The parameters to be identified are summed in table 1.

Parameters	
Symbol	**Description**
$VHC{=}\rho_s c_s$	Volumetric heat capacity of the catalyst
h	Convective heat transfer coefficient
h_{out}	Heat transfer coefficient with ambient
K_{reac}	Scaling factor for $\dot{Q}_{reac}$
s	Slope for the TWC efficency function
$T_{light-off}$	Light-off temperature

Table 1. Parameters to be identified.

The volumetric heat capacity VHC and the heat transfer coefficients h and h_{out} are related to physical proprieties of the catalyst such as material and geometry. K_{reac}, s and $T_{light-off}$ are related to the effects of the chemical reactions occurring in the TWC. Since the only way to test the catalyst was during vehicle operation in the chassis dyno cell, isolating the effect of each parameter on the catalyst temperature response was impractical. In fact, during normal vehicle operation the light-off temperature is reached very quickly after the engine is started and it is not possible to clearly distinguish between the thermal dynamics of the heat exchanged with the exhaust gas and the heat produced by chemical reactions. For this reason all the parameters have been identified simultaneously from the same data set.

The identification procedure finds the optimal set of parameters that minimize a function of the error between the simulated catalyst temperature $T_{cat-sim}$ at the sensor location and the actual measured catalyst temperature $T_{cat-meas}$. The data set used for identification is the combination of a cold start test (figure 6) and an urban driving cycle (figure 7). Including the cold-start test in the identification data set turned out to be necessary since parameters like $T_{ligth-off}$ and s play an important role only during the catalyst warm-up but do not influence the temperature response thereafter.

The cost function J to be minimized during the optimization is the summation of the error computed during the cold start and over a driving cycle:

$$J = RMS(e)_{cold-start} + RMS(e)_{driving-cycle} \tag{8}$$

where:

$$RMS(e) = \sqrt{\frac{1}{N_{sample}} \sum_{k=1}^{N_{sample}} (T_{cat-sim}(k) - T_{cat-meas}(k))^2} \tag{9}$$

Furthermore, in order to guarantee that the light-off period has a significant effect on the cost function, the catalyst light-off period was extended as much as possible. This was done by advancing the spark timing with respect to the baseline calibration strategy in order to keep the exhaust temperature relatively low during the first seconds of engine operations.

The simultaneous identification of six parameters represents an optimization problem with a very wide search space. A Particle Swarm Optimization (PSO) algorithm was used to find the parameters because it showed good performance in optimization problems with a wide search area despite its simple structure (Ebbesen et al., 2012). The Matlab implementation of the PSO algorithm presented in Ebbesen et al. (2012) is used in this work. The performance of the PSO algorithm can depend on the initial parameter estimates. The catalyst specifications and geometries are used to compute an initial staring point for physics related parameters while for $T_{light-off}$ and s an initial state is derived from experimental results presented in literature (Kang et al., 2014). Figures 6 and 7 show the identifications results on the cold start and driving cycle respectively.

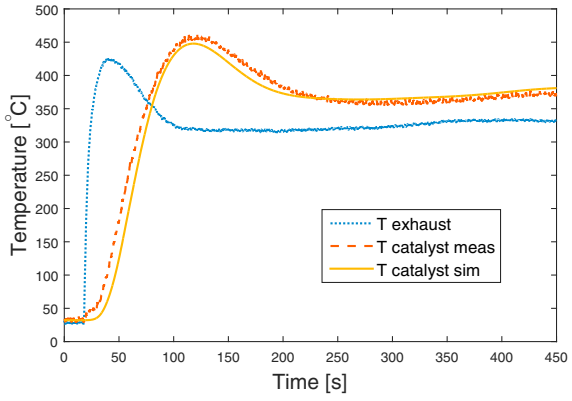

Fig. 6. Identification results on the cold-start test

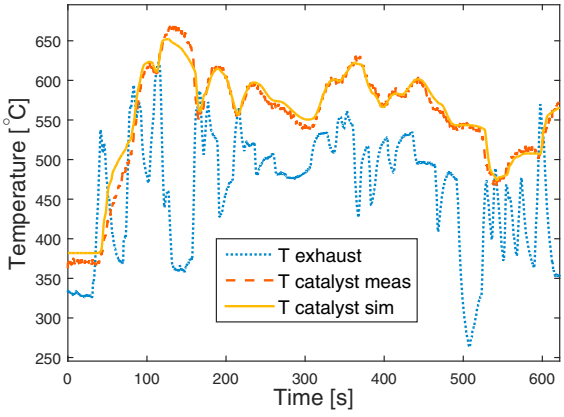

Fig. 7. Identification results on an urban driving cycle test

6. MODEL VALIDATION AND DISCUSSION

The model has been validated with a different data set from the one used for identification. Figure 8 shows the response of the model simulated on an highway driving cycle. The simulation results exhibit very good agreement with the experimental data.

There are some situations in which the model cannot accurately estimate the catalyst temperature. These situations are more prevalent in the urban driving cycle of figure 7 and they are highlighted in figure 9 and 10 together

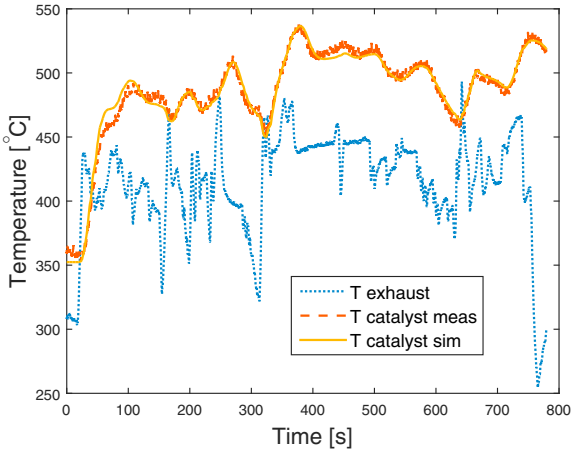

Fig. 8. Model Validation on an highway driving cycle test

with the lambda measurements. From seconds 40 to 80, the model overestimates the catalyst temperature. During this time period the experimental lambda measured at the inlet of the catalyst deviates significantly from the stoichiometric value (see figure 9). Since the model's heat of reactions does not depend on lambda, the catalyst temperature estimation is expected to lack accuracy when the air fuel ratio is far from the stoichiometric value. Specifically, if the engine is running very rich, there is not enough oxygen in the exhaust to convert all the hydrocarbons and carbon monoxide, reducing the heat from reactions. On the other hand, if the engine is running very lean, there is an excess of oxygen in the exhaust and a lack of HC and CO, reducing the heat produced from the most exothermic reactions in the catalyst. Only more accurate modeling of the heat produced by the chemical reactions can improve catalyst temperature accuracy during these conditions.

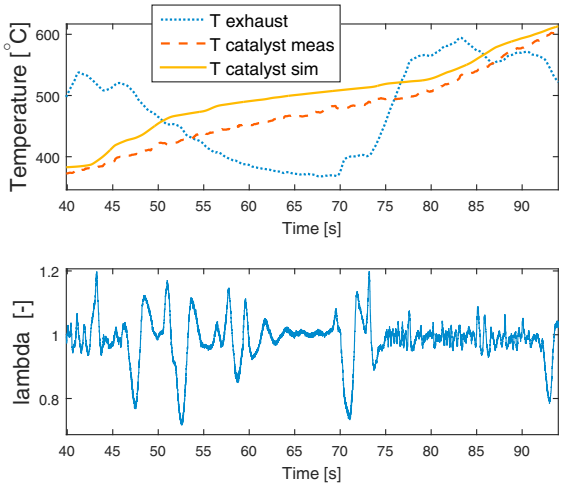

Fig. 9. Overestimation of the temperature when the lambda significantly deviates from stoichiometric

From seconds 120 to 160, the catalyst is in a cooling condition (figure 10). A fuel cut-off occurs (the two lambda sensors saturate at the highest measurable lean value at 120 and 130 seconds). The model is not able to reflect the thermal inertia of the catalyst in this sudden cooling condition. A better characterization of the catalyst solid

phase may improve the catalyst cool-down estimation. For example, considering the external metallic layer and the insulating material as shown in Depcik and Assanis (2005). However, this is not of interest for a control-oriented model.

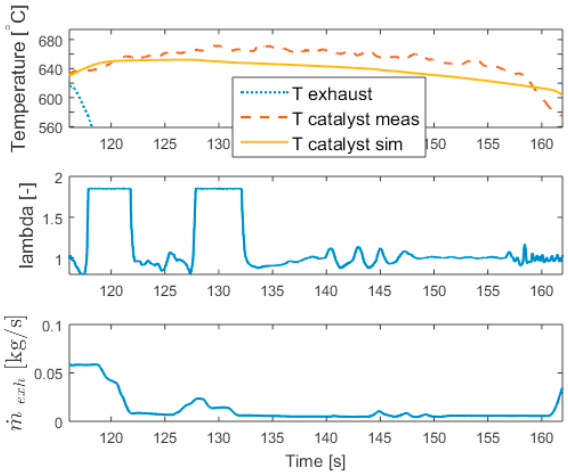

Fig. 10. Catalyst cooling down during fuel cut-off

7. NUMBER OF COMPUTATIONAL NODES

Since the objective is to develop a control-oriented model suitable for real time applications, the complexity of the model must be minimized. For this reason a sensitivity study with respect to the number of computational nodes has been performed with the purpose of analyzing the model's performance when less than 100 computational nodes are considered. Some of the parameters found with the identification procedure described in section 5 (especially K_{reac} and s) have no well defined physical meaning, thus they can be considered lumped parameters representative of complex chemical phenomena. Therefore, the values of these parameters may depend on the number of computational nodes utilized during the identification procedure. In order to perform a meaningful and fair comparison, a new identification of parameters is performed every time the numbers of computational nodes is varied. In figure 11 the cost function value J defined in equations (8) and representative of the model's agreement to the experimental data is shown for different number of computational nodes considered. The results presented in figure 11 show that using more than 10 computational nodes does not lead to any significant improvement in the model accuracy. A number of computational nodes between five and ten can be chosen depending on the accuracy requested by the application.

8. CONCLUSIONS

In this paper a simplified control oriented model of the TWC temperature is derived from PDEs equations describing the catalyst energy balance. The model has been validated with experimental tests reflecting real vehicle operations. The heat produced by the chemical reactions is lumped into a single term so that no concentration information about the species upstream the catalyst is

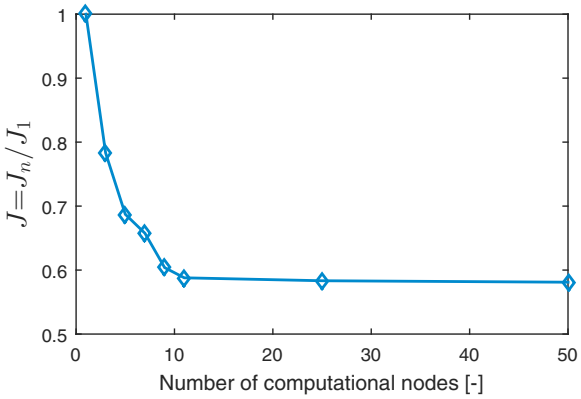

Fig. 11. Model error for different numbers of computational nodes considered. J is normalized with respect to the value computed with a single computational node.

Nomenclature

TWC	Three Way Catalyst	
OSC	Oxygen Storage Component	
PSO	Particle Swarm Optimization	
PDE	Partial Differential Equation	
T_g	gas temperature	$[K]$
T_{cat}	TWC solid phase temperature	$[K]$
$\dot{m}_{exh}$	exhaust gas mass flow rate	$[Kg/s]$
ρ_g	exhaust gas density	$[Kg/m^3]$
ρ_s	TWC solid phase density	$[Kg/m^3]$
c_{p_g}	specific heat of the exhaust gas	$[J/(KgK)]$
c_s	TWC solid phase specific heat	$[J/(KgK)]$
λ_g	exhaust gas conductivity	$[W/(mK)]$
λ_s	TWC solid phase conductivity	$[W/(mK)]$
h	convective heat transfer coefficient	$[W/(m^2K)]$
ϵ	TWC open cross sectional area	$[0-1]$
A_{cs}	TWC cross sectional area	$[m^2]$
A_{geo}	TWC specific geometric area	$[m^2/m^3]$
A_{out}	TWC external surface	$[m^2]$
A_{cat}	TWC specific active surface	$[m^2/m^3]$
V_{cat}	TWC volume	$[m^3]$
D_{cat}	TWC diameter	$[m]$
R_j	reaction rate	$[mol/(m^2s]$
ΔH_j	reaction enthalpy difference	$[J/mol]$
$\dot{Q}_{reac}$	heat produced by reactions	$[W/(m^3)]$

required. Thanks to this approximation, the model is suitable for real time applications like estimation of the light-off temperature during cold start or as support to an OSC model for emission control applications.

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