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A SIMPLIFIED COLDSTART CATALYST THERMAL MODEL TO REDUCE HYDROCARBON EMISSIONS

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Abstract:
It is a well-known phenomenon that the bulk of hydrocarbon emissions emitted from internal combustion engines occurs during the coldstart period, thus necessitating new control strategies to reduce hydrocarbon emissions. A simplified thermal model of the catalytic converter during coldstart is developed, employing thermal dynamics, oxygen storage and static conversion curves. It is subsequently shown that oxygen storage does not play a significant role during coldstart. An empirical parametrization of the catalyst efficiency using Wiebe profiles is proposed to capture general conversion trends of the catalyst. Finally it is shown that the ability of the catalyst to reduce hydrocarbon emissions during coldstart is dominated by its thermal behavior and ability to rapidly achieve lightoff. Model predictions are compared to experimental results for catalyst warmup with good agreement.

Keywords: Automobiles, Air Pollution, Automotive Control, Automotive Emissions, Control Oriented Models, Engine Systems, Non-linear Models

1. INTRODUCTION

Beginning in the late 1950's, legislation was enacted to address growing smog and pollution problems, particularly in the greater Los Angeles metropolitan area, as related to Carbon Monoxide (CO), Unburnt Hydrocarbons (HC), and Nitrogen Oxides (NO_x). The three-way catalyst (TWC) was introduced to resolve the above emissions problem. It has been in widespread use since the early 1980's and is still considered the state of the art.

The temperature operation range of the catalyst must be carefully controlled. The catalyst is generally not active below 400C and begins to age rapidly above 800-900C. Above 1000C, severe aging of the catalyst can occur and at temperatures in the range of 1400C, the substrate itself can melt.

An appropriate model of the catalytic converter is a critical element of the controller structure for Hydrocarbon control. It is desirable to obtain all parameter measurements as close as possible to the engine itself to minimize transport delay in the system. Therefore, a simplified model of the catalyst performance in terms of dynamic conversion efficiency during coldstart as a function of the input flow conditions allows estimation of actual tailpipe Hydrocarbon emissions from measured engine output. The general form of this relation can be described by

$$HC_{out} = f\left(T_{exh}\,,\ \phi_{exh}\,,\ \dot{m}_{exh}\,,\ X_{i,exh}\right) \qquad (1)$$

where HC_{out} = tailpipe Hydrocarbon emissions, T_{exh} = catalyst input temperature, ϕ_{exh} = catalyst input equivalence ratio - equal to the inverse of Air/Fuel Ratio (AFR) made dimensionless by stoichiometric conditions, $\dot{m}_{exh}$ = mass flow rate of exhaust, and Xi, exh = emissions concentration at catalyst input, $i = HC, CO, NO_x$.

The goal of this work is to develop a model of catalyst temperature during coldstart. The conversion efficiency of the catalytic converter and hence the tailpipe Hydrocarbon emissions are strongly dependent on catalyst temperature. All data for this work were obtained from a MY1996 Ford 3.0L 4V DOHC Taurus engine.

2. BACKGROUND OF CATALYST MODELLING

There is a significant body of literature describing research conducted on catalyst and catalytic converter modelling. The models developed typically fall into one of the following three categories (Peyton Jones, 2000).

Detailed physical models, based on fundamental chemical and thermofluidic dynamic principles of reacting flows, e.g. (Vonkeman, 1991). These models include the effects of heat and mass transfer in three dimensions and account for the change in composition of the exhaust gases as they continually react with each other in the catalytic environment. They are very complex and the dynamic effects are not fully understood.

Simplified kinetic models of the reactions between the various gas components, as well as the dynamics of gas storage on the catalyst surface, are used as rapid development tools to study the effects of e.g. geometry and cell density. This reduces the complexity of the problem while still providing sufficient accuracy.

Simplified models, based on the assumption that catalyst behavior is dominated by the dynamics of gas storage, and that other kinetics occur over a much shorter, and less significant, timescale. Models of this type consist essentially of a single non-linear dynamic element characterizing the input/ output AFR response, (ie. the storage dynamics), followed by a more conventional static map of conversion efficiency (Brandt, 1997), (Peyton Jones, 1999), and (Peyton Jones, 2000).

2.1 *Detailed Physical Catalyst Models*

These models consider the coupling of the thermal and chemical behavior of the catalyst, requiring simultaneous handling of the mass and energy balance differential equations. Neglecting phenomena like non-uniform flow distribution and other simplifications (Pattas, 1994) result in a 1-dimensional model where the mass and energy balance equations may be simplified to energy equilibrium in the gas phase, energy equilibrium in the solid phase, mass equilibrium in the gas phase, and mass equilibrium in the solid phase. This 1-dimensional model is used as a basis by a variety of authors (Baba, 1996), (Chan, 1999), (Ohsawa, 1998), and (Shen, 1999).

Further simplifications to this model are made by (Glielmo, 1999) and (Laing, 1999), noting that the thermal dynamics are much slower than the chemical dynamics. (Glielmo, 1999) developed special techniques to solve these simplified differential equations in a two-time-scale. In addition, a genetic algorithm purposely designed as an identification procedure to fit the experimental data is used. The two-time-scale concept is expanded by using neuronal networks and genetic algorithms (Glielmo, 2000).

(Baba, 1996) shows that there is a general maldistribution of species concentrations inside a catalytic converter during warm-up. Because of the low wall temperature there is a high concentration of CO and HC in the exhaust gas passing through outer region cells. To simulate this phenomena the 1-dimensional model described above is expanded. The energy balance in the solid phase is considered two-dimensional and includes axial and radial heat conduction, heat transfer between the exhaust gas and the catalytic surface, and heat release due to chemical reactions.

The reaction scheme can be described by the following reactions:

$$CO + 0.5O_2 \rightarrow CO_2 \quad (2)$$

$$C_3H_6 + 4.5O_2 \rightarrow 3CO_2 + 3H_20 \quad (3)$$

$$H_2 + 0.5O_2 \rightarrow H_2O \quad (4)$$

$$CO + NO \rightarrow CO_2 + 0.5N_2 \quad (5)$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \quad (6)$$

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \quad (7)$$

$$9NO + C_3H_6 \rightarrow 3CO_2 + 3H_2O + 4.5N_2 \quad (8)$$

In most of the models the first 5 reactions are used (Baba, 1996), (Ohsawa, 1998), (Chan, 1999), (Glielmo, 1999), (Glielmo, 2000). The total hydrocarbons (THC) are categorized into two representative groups, propylene (C_3H_6) - representative of fast oxidizing hydrocarbons, and methane (CH_4) - representative of slow oxidizing hydrocarbons. The THC are split into 86% C_3H_6 and 14% CH_4 (Baba, 1996), (Ohsawa, 1998), and (Chan, 1999). (Pattas, 1994) and(Shen, 1999) use propane C_3H_8 oxidation instead of methane. In (Ohsawa, 1998) the NO reduction by propylene is included into the reaction scheme. In (Shayler, 1999) different correlations for heat transfer in the exhaust system and catalytic converter are described.

2.2 *Oxygen Storage and Release Submodel*

Oxygen can be stored and released by the Cerium (Ce) in the washcoat of a catalytic converter (normally oxygen is stored during lean engine operation and released during rich conditions). This phenomenon affects the catalyst's behavior especially during vehicle acceleration and deceleration. Furthermore it is known that due to this effect the conversion efficiency of a TWC is higher under periodic small AFR change than under constant AFR. Therefore the chemisorption of oxygen by Cerium in the washcoat is taken into account by several authors (Pattas, 1994), (Ohsawa, 1998), and (Laing, 1999).

2.3 *Simplified Storage and Conversion Modelling*

This type of model is centered around the reduction of the catalyst model to simple first order submodels, including warmup and lightoff characteristics, oxygen storage and static efficiency curves. This type of model is used by (Brandt, 1997), (Peyton Jones, 1999), and (Peyton Jones, 2000). Typical representations of the submodels are highly empirical and based on large amounts of data collected over widely ranging operating conditions.

Justification of these models is provided by the extensive effort required to determine the values of the physical parameters of detailed chemical and thermodynamics based mathematical models (e.g. coefficients for Arrhenius expressions). By the time the necessary model parameters are known, new catalyst technology is already available.

3. CATALYTIC CONVERTER THERMAL MODEL

The catalytic converter model is based on the following three submodels:

Oxygen storage mechanism= $f(\phi_{exh})$

Efficiency curves= $f(\phi_{exh}, T_{cat})$

Thermal dynamics= $f(T_{exh}, \eta_i, X_{i,exh})$

with T_{cat} the bulk temperature of the catalyst monolith and η_i the catalyst efficiency for the various pollutants as depicted in Figure 1. This basic structure is used as a framework for the model and all submodels are developed based on physical principles and observed phenomena.

3.1 *Coldstart Oxygen Storage*

The Oxygen storage potential of a catalytic converter is well-known and widely reported in the literature. A general methodology has been developed that allows the evaluation of the adsorption and release of oxygen from the catalyst washcoat by looking at the relative amount of Oxygen stored on the surface of the catalyst. Once the washcoat is saturated, the adsorption rate tends to zero while the potential for the release of Oxygen approaches one. As the Oxygen in the washcoat is depleted, this effect is reversed as can be seen in Figure 2 (Brandt, 1997).

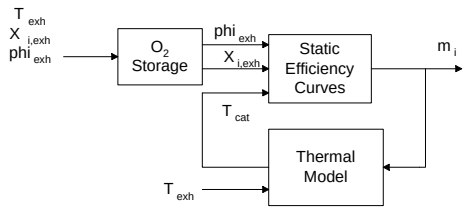

Fig. 1. Catalytic Converter Model Structure

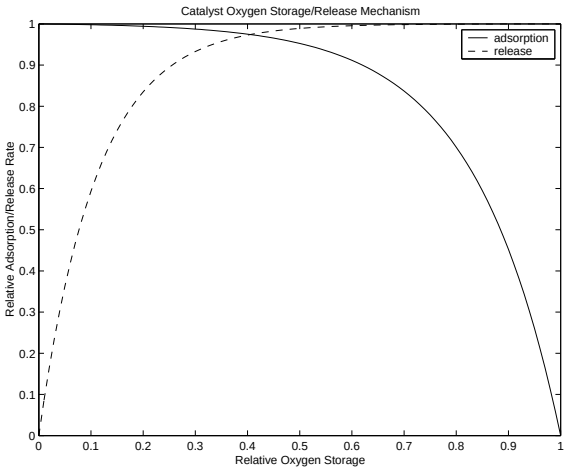

Fig. 2. Catalyst Relative Oxygen Storage.

However, engine tests show the storage and release of Oxygen is not important at coldstart conditions as seen in Figure 3. Although there is a slight storage of Oxygen at very low settings of the idle air control valve, the overall effect of Oxygen storage is small for these conditions.

The reason for this behavior can be explained by two operating conditions. Typically rich operation of the engine during coldstart results in little oxygen in the exhaust for the catalyst to store. Also, the O_2 storage mechanism, which is based on a relative absorption / desorption mechanism, is dependent on transient AFR excursions over the range of operation of the engine which is not applicable at coldstart under relatively steady-state operation. It is also unclear whether the oxygen storage sites in the catalytic converter are active during coldstart conditions.

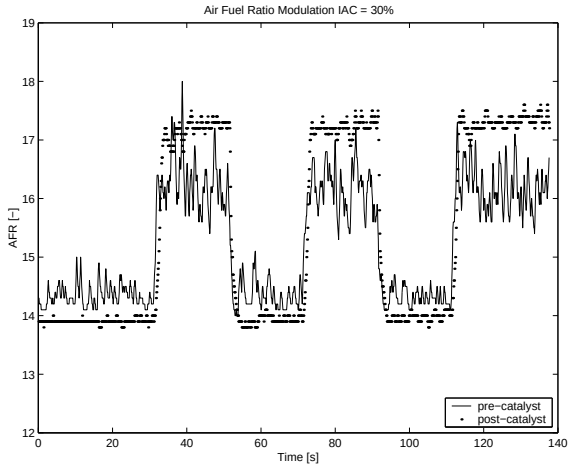

Fig. 3. Catalytic Converter Coldstart Oxygen Storage. IAC = 30%

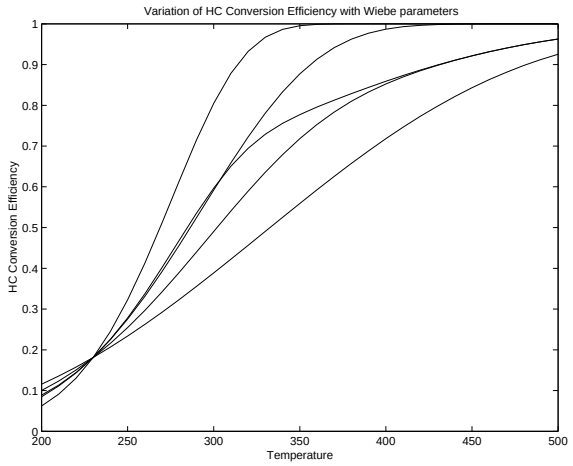

Fig. 4. Catalyst HC conversion efficiency as Wiebe parameters are varied

3.2 *Steady State Conversion Efficiency*

The conversion efficiencies, η_i, are generally measured over a range of temperature T and ϕ, requiring extensive data fitting and/or lookup tables. However, the conversion efficiency can be described by the "S" -shaped Wiebe function with a minimal amount of data collection necessary to describe the conversion trends of the catalyst.

$$y = 1 - exp\left[-a(\frac{u-u_0}{\Delta u})^m\right] \tag{9}$$

where u_0 is the ordinate at y = 10% and Δu the difference in u from e.g. y = 90% to y = 10%, a and m are fitting parameters. In this case , we fit the 50% conversion point, catalyst lightoff. The variation of the Wiebe profile with different combinations of these parameters can be seen in Figure 4, elucidating the ability of this method to fit experimentally observed catalyst efficiency curves.

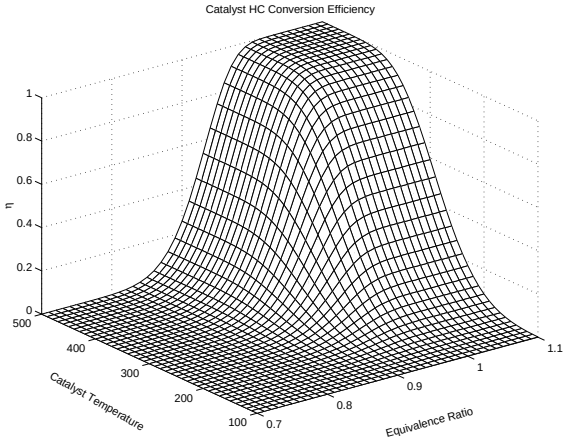

Fig. 5. Efficiency Curve in 2 dimensions as function of T and ϕ

This relation can be extended to two dimensions with the Wiebe representation of η in terms of T and ϕ :

$$\eta_i = 1 - exp\left[-a_1(\frac{\phi-\phi_0}{\Delta\phi})^{m_1} - a_2(\frac{T-T_0}{\Delta T})^{m_2}\right] \tag{10}$$

yielding a contour plot of $\eta = f(\phi, T)$ as shown in Figure 5.

As we are considering idle operation, the variation of $\dot{m}_a$ is small to avoid idle speed fluctuation and it is therefore assumed the dependency of the catalyst conversion on $\dot{m}_a$ is weak. It should be noted that $\dot{m}_a$ must be adjusted as spark timing is retarded to maintain a steady idle speed.

3.3 *Catalytic Converter Thermal Dynamics*

These results lead to the following catalytic converter warmup model dominated by its thermal dynamics and the heat flux within the catalytic converter during startup aimed at determining the temperature in the middle of the catalytic converter as a function of the temperature at the engine outlet, the exhaust mass flow, emissions concentrations, and the air fuel ratio.

A lumped thermal model is used based on engine test results shown in Figure 6. The thermocouples are positioned at the cylinder exhaust, in front of the catalytic converter, and at equi-distant locations throughout the catalytic converter. The engine is run at different steady state operating points of the engine map.

The 1^{st} Law of Thermodynamics applied to the catalytic converter yields the following relationship for the heat transfer to and from the catalytic converter, $\dot{Q}_{cat}$

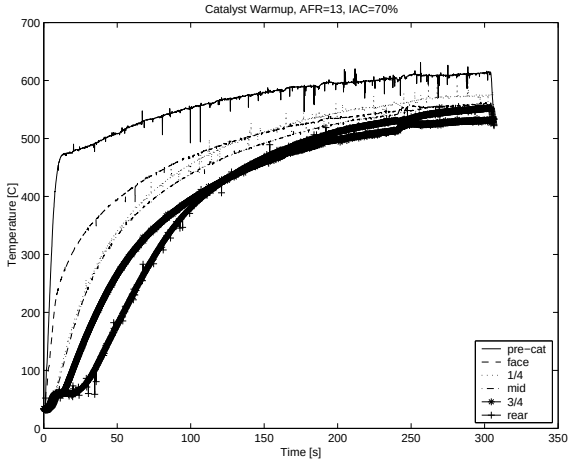

Fig. 6. Temperature Distribution of Catalytic Converter. IAC = 70%

$$\dot{Q}_{cat} = mc_p \frac{dT_{cat}}{dt} = \dot{Q}_{gen} + \dot{Q}_{in} + \dot{Q}_s \qquad (11)$$

where m is the catalytic converter mass and c_p its specific heat at constant pressure.

$\dot{Q}_s$ = heat transfer to the surroundings

$$\dot{Q}_s = h_s A(T_{atm} - T_{cat}) \qquad (12)$$

where h_s is the heat transfer coefficient from the catalytic converter to the surroundings, A is the catalyst effective area, and T_{atm} the ambient temperature. This is determined experimentally by catalyst cooldown tests with the engine not operating, assuming no radiation or conduction.

$\dot{Q}_{in}$ = heat transfer due to exhaust enthalpy flow into catalyst

$$\dot{Q}_{in} = h_{in} A(T_{exh} - T_{cat}) \qquad (13)$$

with h_{in} being the internal heat transfer coefficient. This can be determined experimentally by catalyst warmup tests under rich operation (no oxidation energy inside catalyst) as shown in Figure 7. The total heat transfer coefficient for the catalytic converter is shown in Figure 8.

$\dot{Q}_{gen}$ is the heat generated by conversion of pollutants in the catalytic environment and can be calculated as follows, modelling THC as 86% propylene and 14% methane, in accordance with the literature.

$$\dot{Q}_{gen} = \dot{n}_{converted} \Delta H_{gen} \qquad (14)$$

$$= \sum_i \eta_i X_i \left(\frac{\dot{m}_a (1 + \frac{\phi}{AFRst})}{M_{exh}} \right) \Delta H_{i,gen} \qquad (15)$$

where n_i is the number of moles of pollutant converted in the catalyst and ΔH_{gen} the corresponding heat of formation. M_{exh} is the average molecular weight of the exhaust. Accounting for the conversion of HC and CO in the catalyst during coldstart, the heat generation is now

$$\dot{Q}_{gen} = \frac{\dot{m}_a (1 + \frac{\phi}{AFR_{stoich}})}{M_{exh}} * [\eta_{CO} X_{CO} \Delta H_{CO} + \eta_{HC} X_{HC} (0.86 \frac{\Delta H_{C_3H_6}}{3} + 0.14 \Delta H_{CH_4})] \qquad (16)$$

The strong dependency of catalyst temperature on $\dot{m}_{exh}$ is mitigated by the relatively small variation of $\dot{m}_a$ in order to maintain a steady idle speed. In general, however, increasing the engine speed and thus increasing $\dot{m}_{exh}$ has a large effect on the temperature of the catalyst and its increase over time during the coldstart period.

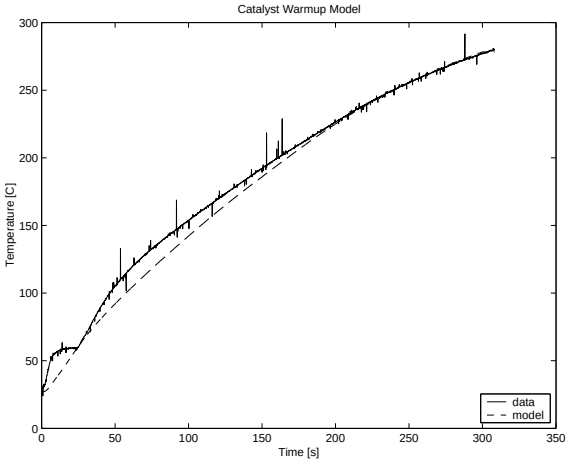

Fig. 7. Catalytic Converter Warmup under Rich Coldstart Conditions.

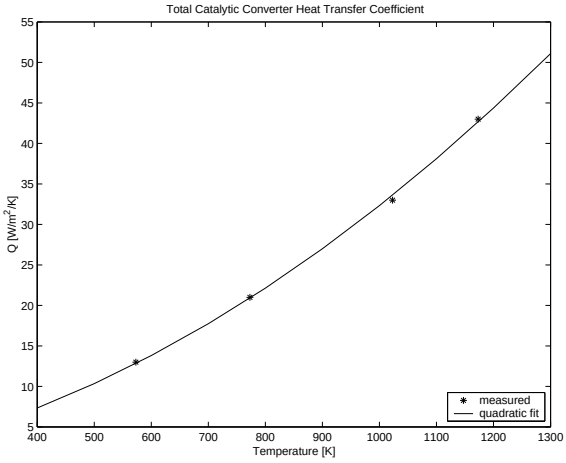

Fig. 8. Catalytic Converter Total Heat Transfer

4. CONCLUSION

The warmup of the catalytic converter during the coldstart period is a critical factor in the overall production of hydrocarbon emissions from an

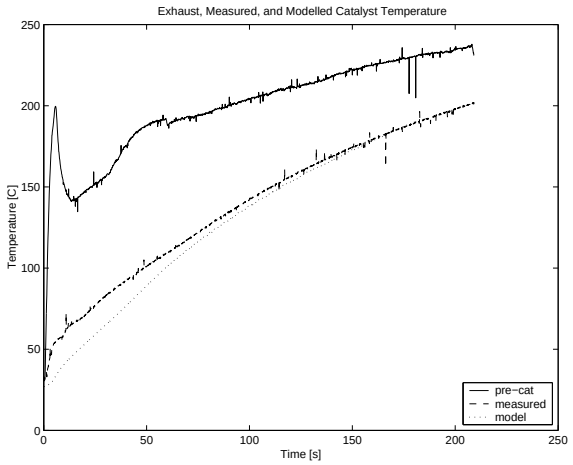

Fig. 9. Measured and Predicted Catalyst Thermal Behavior

automobile. The catalytic material is generally not active at low temperatures and it is therefore necessary for the catalyst to achieve lightoff temperatures in as short a time as possible.

A simplified thermal model of the catalyst is developed that requires a minimal amount of data collection for parameter fitting. The temperature of the catalytic converter is shown to depend primarily on the amount of pollutants oxidized from the exhaust stream, the exhaust gas temperature entering the catalytic converter, and heat transfer to the surroundings. The oxygen storage potential of the catalyst during coldstart is shown to be minimal. A comparison of measured thermal behavior of the catalyst with model predictions is shown in Figure 9 along with the exhaust gas inlet temperature.

Further work is necessary to extend the thermal dynamics of the catalyst to describe the cumulative production of hydrocarbons during the coldstart period. The composition and temperature of the exhaust stream from the engine can be optimized to minimize tailpipe hydrocarbons. The validity of the model is currently being checked against datasets from other engine and catalyst combinations.

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