The Effect of Grid Resolution and Oxygen Storage in a One-Dimensional Monolithic Three-Way Catalyst Model

Denis I. Andrianov ∗ Robert J. Dingli ∗ Michael J. Brear ∗ Chris Manzie ∗

∗ Department of Mechanical Engineering, The University of Melbourne, Victoria 3010, Australia (E-mail: d.andrianov@pgrad.unimelb.edu.au, rdingli@unimelb.edu.au, mjbrear@unimelb.edu.au, manziec@unimelb.edu.au)

Abstract:
A one-dimensional model of a monolithic three-way catalyst is presented, featuring a reduced order chemical kinetic scheme comprised of ten reactions and including oxygen storage. The model behaviour is validated against measurements taken from air/fuel ratio sweeps as well as European emission drive cycle data, covering a broad range of flow velocities, gas composition and inlet temperatures. The effects of grid resolution and oxygen storage reactions are investigated to provide insight into the minimum modelling requirements to capture key phenomena such as light-off time and conversion efficiency of the catalyst.

Keywords:
Reduced-order models, automotive emissions, engine control, optimisation problems

1. INTRODUCTION

The major pollutants from vehicles with internal combustion engines are unburned hydrocarbons (HC), carbon monoxide (CO) and oxides of nitrogen (NOx). Tail-pipe NOx emissions are largely comprised of NO and not NO2 (Twigg, 2007). In the atmosphere, in the presence of various unburned hydrocarbons and CO, NO is converted to NO2. Under the influence of light, a fraction of NO2 decomposes back into NO, losing an oxygen atom, which quickly combines with atmospheric oxygen O2, forming harmful ozone O3. NO2 is eventually transformed almost entirely into nitric acid (HNO3) in the form of acid rain, acid fog, or dry deposition (Seinfeld, 2004; Twigg, 2007).

The first attempt to tackle this problem was with the introduction of a catalytic converter in 1975, which helped to cut HC and CO emissions by roughly 96% and NOx emissions by 75% (Seinfeld, 2004). Most of the early catalysts were in pellet form and were soon abandoned due to catalyst wear and subsequent deterioration in their performance. Newer catalytic converters feature a monolithic structure with a large number of long thin channels, the surface of which is coated with a catalytically active material, referred to as a washcoat. Monolithic substrates are often manufactured from cordierite, a ceramic with a very low coefficient of thermal expansion. This helps to prevent cracking of the material when it experiences high temperatures and spatial temperature gradients during normal operation. The washcoat is typically on the order of 20–150 µm thick (Twigg, 2007) and contains a combination of two or more of the following metals: platinum (Pt), palladium (Pd) and rhodium (Rh). A catalyst that can simultaneously remove HC, NOx and CO emissions is called a three-way catalyst (TWC).

For the conversion efficiency to be maximised, TWC’s usually require combustion to take place at close to a stoichiometric air/fuel mixture. Since precisely stoichiometric conditions are difficult to maintain, the washcoat is fitted with some oxygen storage compounds such as ceria (cerium oxides), which absorb oxygen under lean conditions and release oxygen under rich conditions. This mechanism improves the performance of TWC’s by helping to maintain the exhaust around stoichiometric conditions.

During roughly the last 25 years, some significant contribution has been made towards the understanding of the processes within the TWC, its mathematical modeling and simulation. However, many of the available models in the literature are of too high order to be useful for control or optimisation studies. The development of models with appropriate complexity to capture the key characteristics, while remaining suitable for optimisation studies and real time control, is an existing challenge. It is well known that most pollutants are emitted during the first few minutes of driving, while the catalyst is below its activation or light-off temperature. Appropriate models could potentially be used to help minimise tail-pipe emissions over the warm up period by optimally scheduling engine control variables such as the air/fuel ratio, spark timing, cam phasing and throttle angle.

Voltz et al. (1973) was one of the first to formulate the reaction rates on the surface of a platinum catalyst. His work appears to have formed the basis for almost all future developments in this area of research. Voltz’s basic model has since been extended by others with updated
kinetics and more chemical reactions (e.g. Subramaniam and Varma (1985); Dubien et al. (1998); Pontikakis and Stamatelos (2004); Holder et al. (2006)).

One-dimensional TWC models (Heck et al., 1976; Oh and Cavendish, 1982; Groppi et al., 1995; Siemund et al., 1996; Holder et al., 2006) predict the distribution of temperature and species concentration along the length of the catalyst as a function of time. Whilst these models contain a number of simplifying assumptions, some of which are the subject of debate, the use of more complex models would render many optimisation studies infeasible. One of the major drawbacks of 1D models is the need for Nusselt number (Nu) and Sherwood number (Sh) correlations for calculation of the heat and mass transfer coefficients (Hayes and Kolaczkowski, 1994; Groppi et al., 1995; Wanker et al., 2000). Two-dimensional (Hayes and Kolaczkowski, 1994; Groppi et al., 1995; Wanker et al., 2000) and three-dimensional (Groppi et al., 1995; Jeong and Kim, 2001) models also exist, but require a substantial amount of computation time.

A relatively simple one-dimensional TWC model formulation is presented in this paper, the solutions of which are comparable to accurately resolved one-dimensional models. While still incorporating a chemical kinetic scheme, the model is adequate for many optimisation studies, demonstrating reasonable estimates of light-off time and tail-pipe emissions.

2. MODELLING

A one-dimensional model is considered in this work. The model is based heavily on previous 1D models and separates the conditions inside the washcoat layer from the bulk fluid conditions inside the channels.

2.1 Key Model Characteristics

No heat loss from the monolith to the environment is considered. All properties of the solid phase are constant, except the temperature. A uniform flow distribution is assumed across the face of the monolith block. Non-uniformities are therefore accounted for in the model optimisation which effectively averages across all channels. Reactions occur within the washcoat layer, and heat is generated at the interface between the solid and gas phases.

The gas pressure along the length of the monolith is assumed to be at atmospheric pressure. The density of the exhaust is therefore a function of temperature only. Laminar flow is assumed since the hydraulic diameter of monolithic channels is small and the Reynolds number based on the diameter ranges from about 20 to 400.

Axial thermal conduction in the solid phase is considered. Axial thermal conduction in the gas phase is ignored as convective heat transfer dominates in the stream-wise direction under mean flow velocity. The heat transfer between the gas and solid phases is governed by forced convection. Mass transfer between the gas and solid phases is governed by diffusion. The diffusion velocities of all species are expected to be much smaller than the average flow velocity and, hence, axial species diffusion in the gas phase is ignored.

| Table 1: Variables defining a TWC model |
| Var. | Description | Value |
| S | geometric surf. area per reactor vol. | 2740 m²/m³ |
| a* | catalytic surf. area per reactor vol. | 548 m²/m³ |
| ρ | reactor void fraction | 0.757 |
| ρs | density of the substrate | 2240 kg/m³ |
| kq | thermal conduct. of the substrate | 3.0 W/m·K |
| CPs | specific heat capacity of the substrate | 900 J/kg·K |
| ψ* | oxygen storage capacity | 150 mol/m³ |
| l̃w | washcoat thickness | 17 × 10⁻⁶ m |
| L | reactor length | 0.1435 m |
| D참 | hydraulic diameter of channels | 0.0011 m |

2.2 Model Equations

The parameters defining the model are given in Table 1. Let $h_{gs}$ and $h_{m,gs,i}$ denote heat and mass transfer coefficients of species $i$, $R_{eq,i}$ the consumption rate of species $i$, $R_{eq,j}$ the rate and $\Delta h_{r,j}$ the enthalpy of reaction $j$ in the washcoat for a total of $N$ reactions. Also let $M_S$, $C_{P,g}$, $ρ_g$ and $u$ be the molar mass, specific heat capacity, density and velocity of the exhaust gas respectively. The equations for the fluid temperature $T_g$, the substrate temperature $T_s$, the molar fractions of species $i$ in the flow $C_{g,i}$ and inside the washcoat layer $C_{s,i}$ can be described as

\[ \frac{\partial T_g}{\partial t} = -\rho_g C_{P,g} \frac{\partial T_g}{\partial x} + R_{eq,g}(T_g - T_g), \]  

\[ C_{P,g} \rho_g (1 - \epsilon) \frac{\partial T_s}{\partial t} = k(q_s)(1 - \epsilon) \frac{\partial^2 T_s}{\partial x^2} + h_{gs}(T_g - T_s), \]  

\[ h_{gs}(T_g - T_s) = \sum_{i=1}^{N} R_{eq,j} \Delta h_{r,j}, \]  

\[ \frac{\partial C_{g,i}}{\partial t} = -u \frac{\partial C_{g,i}}{\partial x} - h_{m,gs,i}(C_{s,i} - C_{g,i}), \]  

\[ \rho_g h_{m,gs,i} \frac{\partial C_{s,i}}{\partial t} = \sum_{j=1}^{N} R_{eq,j} S_{\frac{C_{g,i} - C_{s,i}}{\Delta h_{r,j}}} - \alpha M_S R_{eq,i}. \]

The reactions considered and the corresponding indices $j$ from 1 to 10 are

(1) $CO + 0.5O_2 \rightarrow CO_2$
(2) $H_2 + 0.5O_2 \rightarrow H_2O$
(3) $CH_{fast} + 1.45O_2 \rightarrow CO_2 + 0.9H_2O$
(4) $CH_{slow} + 1.45O_2 \rightarrow CO_2 + 0.9H_2O$
(5) $2NO + 2CO \rightarrow 2CO_2 + N_2$
(6) $C_2O_2 + 0.5O_2 \rightarrow 2CO_2$
(7) $C_2O_2 + NO \rightarrow 2CO_2 + 0.5N_2$
(8) $2CO_2 + CO \rightarrow C_2O_2 + CO_2$
(9) $CH_{fast} + 3.8CeO_2 \rightarrow 1.9CeO_3 + CO_2 + 0.9H_2O$
(10) $CH_{slow} + 3.8CeO_2 \rightarrow 1.9CeO_3 + CO_2 + 0.9H_2O$

and have been taken from Pontikakis and Stamatelos (2004) along with the corresponding reaction rates $R_{eq,j}$, which incorporate oxygen storage dynamics for some fixed oxygen storage capacity $\Psi$. The developers of the chemical kinetic scheme have used a catalyst with precious metal loading of roughly 1770 g/m³ and a $Pt : Rh$ ratio of 5 : 1 in their experiments for tuning the reaction rates. However, our washcoat composition (Table 2) was different. The reactions rates $R_{eq,j}$ have been taken directly from Pontikakis and Stamatelos (2004) and have not been optimised for our catalyst.
Consumption rates \( R_i \) are calculated from these reaction rates. An additional differential equation is included with the reaction scheme,

\[
\frac{d\psi}{dt} = \frac{R_r,6 + R_r,7}{\Psi} - \frac{R_r,8 + R_r,9 + R_r,10}{\Psi},
\]

(5)
capturing the current fraction of oxygen saturation in the washcoat, \( \psi \), at a particular time instant. Two lumped categories of hydrocarbons are considered: quickly oxidising ("fast" HC) and slowly oxidising ("slow" HC), which is common practice in many reduced order chemical reaction schemes (Oh and Cavendish, 1982; Zyguorakis and Aris, 1983; Dubien et al., 1998). The relative amount of engine-out fast and slow HC is difficult to predict or measure. This ratio is therefore fixed. The enthalpies of reaction \( \Delta h_{r,j} \) are calculated from the enthalpies of formation of relevant species. Cioslowski et al. (2000) and Lide (2007) provide all of the necessary data. The heat and mass transfer coefficients are obtained from

\[
h_{gs} = \frac{k_g}{D_h} N u D_h, h_{m,gs,i} = \frac{D_i}{D_h} S h D_{h,i},
\]

where \( k_g \) is the thermal conductivity of the exhaust gas, and \( N u \) and \( Sh \) are Nusselt and Sherwood numbers. The diffusion coefficients \( D_{i} \) have been obtained from Fuller et al. (1966), and are approximated for a binary mixture of nitrogen and the species in question. Since the exhaust is comprised largely of nitrogen, the thermal conductivity of the exhaust mixture is approximated by

\[
k_g = 2.269 \times 10^{-4} \frac{g \cdot s^2}{C m}
\]

(6)
for nitrogen from Oh and Cavendish (1982). The \( N u \) and \( Sh \) correlations proposed by Hawthorn (1974) are used in this work:

\[
N u D_h = 3.66 \left( 1 + 0.095 \frac{D_h}{L} P e_{ch,D_h} \right)^{0.45},
\]

(7)

\[
Sh D_{h,i} = 3.66 \left( 1 + 0.095 \frac{D_h}{L} P e_{m,D_h,i} \right)^{0.45},
\]

(8)
where \( P e \) are Peclet numbers, defined as

\[
P e_{ch,D_h} = R e_{D_h} P r, \ P e_{m,D_h,i} = R e_{D_h} S c_i.
\]
The terms \( Pr, Sc \) and \( Re \) are Prandtl, Schmidt and Reynolds numbers respectively, formulated as

\[
Pr = \frac{C_{P,eff} \mu}{k_g}, \ Sc_i = \frac{\mu}{\rho_g D_{i,N}}, \ Re_{D_h} = \frac{\rho_g u D_h}{\mu},
\]

where \( \mu \) is the dynamic viscosity of the exhaust.

2.3 Boundary Conditions

Given that \( T_g^{in} \) is the gas temperature and \( C_{i}^{in} \) are the molar fractions of species \( i \) at the inlet of a TWC, the boundary conditions are

\[
T_g(0, t) = T_g^{in},
\]

(9)

\[
C_{g,O_2}(0, t) = C_{g,O_2}^{in},
\]

(10)

\[
C_{g,CO}(0, t) = C_{g,CO}^{in},
\]

(11)

\[
C_{g,H_2}(0, t) = \frac{1}{3} C_{g,CO}^{in},
\]

(12)

\[
C_{g,N_2}(0, t) = C_{g,N_2}^{in},
\]

(13)

\[
C_{g,HC_{fast}}(0, t) = 0.85 C_{g,HC}^{in},
\]

(14)

\[
C_{g,HC_{slow}}(0, t) = 0.15 C_{g,HC}^{in},
\]

(15)

\[
\frac{\partial C_{g,i}}{\partial x} \bigg|_{x=L} = 0.
\]

(16)

According to Pontikakis and Stamatelos (2004) the dynamics of the water–gas shift reaction

\[
CO + H_2O \rightarrow CO_2 + H_2
\]

result in the content of \( CO \) being roughly equal to a third of \( CO \). This approximation was used as \( H_2 \) concentrations at the inlet could not be measured with the available lab equipment. The split between fast and slow-oxidising hydrocarbons (14)–(15) was also adopted from Pontikakis and Stamatelos (2004).

2.4 Solution Scheme

The partial differential equations (1)–(4) were discretised using central differences. The spatial domain was divided into a uniform grid of resolution \( \Delta x \). The variables \( T_g, T_s, C_g \) and \( C_s \) were resolved using 51 (\( \Delta x = 2.81 \ mm \)), 2 (\( \Delta x = 71.75 \ mm \)) and 1 node (\( \Delta x = 35.875 \ mm \)).

With such discretisation, equations (1)–(4) are reduced to a system of ODE’s, \( \dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), t) \), with 15 differential equations associated with each node. The presence of reaction kinetics that are highly sensitive to temperature and reactant concentrations introduces numerical stiffness. A stiff implicit solver, DASSL, developed in Petzold (1982) was chosen for the development of solutions.

If the lumped parameter model (1 node) is allowed to span the entire length of the catalyst, such that \( \Delta x = 143.5 \ mm \), the thermal mass of the element becomes so large that the substrate temperature can be affected considerably during warm-up. This in turn can lead to significant errors in the prediction of light-off time, and hence, overall tail-pipe emissions. It has been empirically determined that by constraining \( \Delta x \) to 1/4 of the brick’s length, the performance of the lumped parameter model (1 node) was closest to that of the models with a higher spatial resolution. This was possible as most \( CO, NO \) and \( HC \) molecules are consumed in front portion of the monolith.

The amount of computation time spent on a 1.80 GHz Pentium 4 computer was roughly 20 hours for a 51 node, 3 min 30 sec for a 2 node and 45 sec for a 1 node discretisation scheme over 600 seconds of the NEDC test conditions. Note that whilst the accuracy of the model appears to be reduced only slightly, as the spatial grid resolution is dropped from 51 to 2 nodes, the amount of computational effort is reduced substantially. Further
model simplification with the omission of oxygen storage reactions gave a simulation speed improvement of roughly a third.

3. EXPERIMENTAL WORK

Experiments were conducted on a 4 litre Ford BF engine and a Horiba-Schenck Titan 460 kW transient dynamometer. The equipment was controlled remotely using ATI Vision and STARS software packages. Experimental data was acquired using the same software.

The exhaust system was comprised of a cast iron exhaust manifold, front pipe, an adaptor joining the front pipe to the exhaust manifold and slightly modified inter and rear pipes to suit the test cell’s spatial constraints. The front, inter and rear pipes were standard Ford components. The set up is shown in Figure 1 along with locations of various sensors.

The TWC was aged in a 75 hour Ford 4-mode schedule, equivalent to ≈ 80000 km. Its properties are outlined in Table 2. Three equally spaced thermocouples were inserted into the monolith. Two more thermocouples were placed directly before and after the catalyst to measure inlet and exit gas temperatures.

A Cambustion HFR400 Fast Flame Ionisation Detector (FFID) measured pre-catalyst and post-catalyst HC emissions. This device has a time constant of less than 2 ms and is specifically designed for taking measurements in the exhaust system where significant pressure fluctuations can exist. Two Autodiagnostics ADS9000 gas analysers were employed to measure pre-catalyst O\textsubscript{2}, CO, CO\textsubscript{2}, NO and HC, and post-catalyst O\textsubscript{2}, CO, CO\textsubscript{2} and HC. Tail-pipe NO emissions were not measured. The ADS9000 uses non-dispersive infrared (NDIR) techniques to measure CO, CO\textsubscript{2} and HC and an electro-chemical cell method to measure O\textsubscript{2} and NO\textsubscript{X} emissions. It samples at a rate of roughly 1.4 Hz and has a time constant on the order of a few seconds.

Normalised air/fuel ratio (λ) measurements were taken using a Bosch LSU4.9 wideband oxygen sensor (UEGO) and the fuel flow rates were measured using an AVL KMA 4000 fuel conditioning system. Mass flow rates in the exhaust were then calculated from these two measurements.

This paper presents results from two experimental test cases. One is based on the first 600 seconds of the New European Drive Cycle (NEDC) operating conditions (engine speed and torque), logged in a vehicle chassis dynamometer test and implemented on the engine dynamometer (see Figure 2). The engine operated using an existing control strategy, and thus for the majority of the time λ ≈ 1. A zoomed in view of λ around light-off is given in Figure 3.

The second test was a custom cycle, performed over 600 seconds from a cold start with a constant pedal position and engine speed fixed at 1500 RPM. The torque produced was in the range 70–150 Nm, depending on the λ setpoint. During the first 300 seconds λ ≈ 1, while the remainder of the test is identified by a pulsating λ as shown in Figure 4. This alters the feed gas composition and provides the model with an extended validation case. The mass flow rates in this test were up to 5 times higher than in the NEDC test.

### Table 2. Physical Properties of the TWC

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substrate material</td>
<td>Cordierite</td>
</tr>
<tr>
<td>Channel shape</td>
<td>Square</td>
</tr>
<tr>
<td>Number of bricks</td>
<td>1</td>
</tr>
<tr>
<td>Length</td>
<td>143.5 mm</td>
</tr>
<tr>
<td>Channel hydraulic diameter</td>
<td>1.105 mm</td>
</tr>
<tr>
<td>Thickness of channel walls</td>
<td>0.165 mm</td>
</tr>
<tr>
<td>Cross-sectional area</td>
<td>0.0119 m²</td>
</tr>
<tr>
<td>Pt : Pd : Rh composition</td>
<td>12:0:5</td>
</tr>
<tr>
<td>Loading</td>
<td>600 g/m³</td>
</tr>
</tbody>
</table>

Fig. 1. Exhaust system

Fig. 2. NEDC drive cycle

Fig. 3. λ shortly before and after light-off (NEDC)
in Pontikakis and Stamatelos (2004). These values seem reasonable, given that our aged catalyst (Table 2) has a precious metal loading of roughly a third of that of Pontikakis and Stamatelos (2004). The parameter $\alpha$ is expected to be a fraction of $S$ as it takes into account catalyst three-dimensionality and the reduction in the active surface area due to ageing.

4. RESULTS

A comparison between the measured and the estimated instantaneous tail-pipe emissions is made in Figures 5 and 6. Here the model was discretised using 51 nodes or a grid resolution of $\Delta x = 2.81$ mm. It can be seen that measured and estimated post-catalyst concentrations do not always agree, but most trends are well captured. This is typical behaviour of 1D catalyst models, as Pontikakis and Stamatelos (2004) showed.

Consider the NEDC test results of Figure 5. Early CO and HC light-off is predicted by the model roughly 85 seconds into the drive cycle. At this instant the model predicts a substrate temperature of 545 K at 1/4 length from the inlet, while the temperature measurement is 560 K for the same position (Figure 7). Modelled and measured temperatures compare well before the predicted light-off. However, actual light-off occurs only when the measured temperature approaches 620 K at 147 seconds. It may be argued that the light-off temperature could have been lower than this, as a rich discharge occurred shortly before light-off, between 143 and 147 seconds, with $\lambda$ dropping to as low as 0.8 (see Figure 3), inhibiting possible oxidation reactions. This part of the cycle corresponded to a rapid throttle closing event and poor mixture control. The TWC temperature climbed from 590 K to 620 K. Thus, the true light-off temperature for $\lambda = 1$ is expected to lie within this range. The discrepancy between the predicted and the measured light-off temperature for $\lambda = 1$ is expected to be due to either catalyst aging, the differing $Pt : Rh$ ratio used in this work and that of Pontikakis and Stamatelos (2004) or both.

Consider instantaneous emission results from the second test case in Figure 6. The light-off time is observed 43 seconds into the test and is predicted well. By $t = 43$ s the modelled temperature at 1/4 length position from the inlet was 650 K, coinciding with the measured temperature (Figure 8). This light-off temperature is significantly higher than what was observed in the NEDC cycle.
High mass flow rates prevail in this test case and at the previously modelled light-off temperature of 545 K the consumption rates are not fast enough to remove the additional inflow of CO and HC molecules. As a result a large proportion of CO and HC pass the front of the monolith unreacted. Substrate temperatures downstream are much lower and CO and HC react much less there. The light-off is thus postponed until higher substrate temperatures, and thus, faster reaction rates are achieved. A better prediction of the light-off time is a consequence of a much quicker substrate temperature rise compared to the NEDC test case.

To compare the performances of the catalyst models of various grid resolutions, consider the results from the NEDC test in Figure 9 and the custom cycle in Figure 10. A very good agreement is demonstrated between the solutions using a fine (51 node), and an extremely sparse (2 node) grid. This observation was at first surprising to the authors, but the distribution of consumption rates \( R_{c,i} \) [mol/(m\(^3\) \cdot s)] in the 2 node model under many conditions appear to sensibly approximate those in the 51 node model. The lumped parameter model performs notably worse, but most trends are still followed.

Figures 11 and 12 demonstrate measured and simulated, using various number of nodes, cumulative emissions over the two test cycles. It can be seen that cumulative emissions compare much better than instantaneous emissions from Figures 5 and 6 for all model discretisation schemes.

The effect of removing all oxygen storage reactions from the chemical kinetic scheme on instantaneous post-catalyst emissions is demonstrated in Figure 13 for the NEDC test case (modelled with 51 nodes). Comparisons of cumulative emissions are shown in Figure 14. It can be seen that the conversion efficiency of CO is almost unaffected, while that of HC is considerably degraded. This is because under this kinetic scheme and test conditions, almost all CO and fast-oxidising HC are oxidised via reaction 1 and 3 mechanisms respectively, while oxidation via reaction 8 and 9 is limited. However, slow-oxidising HC are primarily oxidised by reaction 10, and the removal of oxygen storage reactions 6–10 heavily restricts their oxidation in simulations. Similar observations have been reported (Shamim et al., 2002; Shamim, 2008) with other kinetic schemes.

5. CONCLUSION

One of the major requirements for solving dynamic optimisation problems are models with the minimum number of state variables. A representation of a TWC model with a small ODE system was identified in this paper, making such optimisation studies possible.

This paper demonstrated that with reasonable accuracy a one-dimensional TWC model may model the light-off time and tail-pipe emissions. The performance of the models with 2 and 51 nodes is very similar, whilst the results of simulations using the lumped parameter model are comparable. A simplification of the chemical kinetic scheme via the removal of oxygen storage reactions leads to an underestimation of HC conversion efficiency. However, the light-off time can still be adequately predicted.
Fig. 10. Effect of grid resolution on the modelled tail-pipe (a) CO, (b) HC molar fractions in the 2nd test

Fig. 11. Measured and modelled tail-pipe (a) CO, (b) HC cumulative emissions over the NEDC

Fig. 12. Measured and modelled tail-pipe (a) CO, (b) HC cumulative emissions in the 2nd test

Fig. 13. Effect of oxygen storage reactions on post-catalyst (a) CO, (b) HC molar fractions over the NEDC
Fig. 14. Effect of oxygen storage reactions on post-catalyst (a) CO, (b) HC cumulative emissions over the NEDC

ACKNOWLEDGEMENTS

This research was supported by the Advanced Centre for Automotive Research and Testing (ACART, http://www.acart.com.au).

REFERENCES


