

Modelling the effect of moisture on catalyst warm-up

Clarkson, R.J. & Benjamin, S.F.

Published version deposited in CURVE July 2013

Original citation & hyperlink:

Clarkson, R.J. and Benjamin, S.F. (1995) 'Modelling the effect of moisture on catalyst warm-up. In *Proceedings of IMechE/SAE VTMS2 Conference*. London: IMechE.

<http://www.imeche.org/>

Copyright © and Moral Rights are retained by the author(s) and/ or other copyright owners. A copy can be downloaded for personal non-commercial research or study, without prior permission or charge. This item cannot be reproduced or quoted extensively from without first obtaining permission in writing from the copyright holder(s). The content must not be changed in any way or sold commercially in any format or medium without the formal permission of the copyright holders.

CURVE is the Institutional Repository for Coventry University

<http://curve.coventry.ac.uk/open>

Modelling the Effect of Moisture on Catalyst Warm-Up

R J Clarkson and S F Benjamin
Coventry University, UK

SYNOPSIS The presence of moisture in exhaust systems is identified as being responsible for temperature plateaux that occur during the early stages of catalyst warm-up. A mathematical representation of the associated condensation-evaporation processes is developed, and is shown to give good agreement with experimental data. It is demonstrated that these processes only have a significant effect on light-off times and mass of emissions species discharged if the catalyst lights-off towards its rear.

NOTATION

a_v	ratio of monolith area to monolith volume
c_{gw}	mass fraction of moisture in exhaust gas
c_{ps}	specific heat capacity of monolith
C_{sw}	concentration of water in washcoat
C_{sw}^o	concentration of water in washcoat at previous time step
D_w	diffusivity of moisture in exhaust gas
h_{fg}	latent heat of vaporisation
K_{mv}	moisture mass transfer coefficient
t	time
U	channel velocity
v'_{sw}	specific volume of saturated water vapour
x	axial position along monolith
α	monolith free volume
ρ_g	exhaust gas density
Θ_s	temperature of monolith in °C

1 INTRODUCTION

Mathematical models of automotive catalytic converters have been recognised as valuable analytical tools for many years; since the early 1970's numerous attempts have been made to develop such models for monolith type catalysts [1]. For a model to achieve a high level of generality it has to be based on mathematical relationships of such complexity a numerical approach is required to obtain solutions. Although most of the existing models of this type are capable of reliable qualitative predictions, accurate quantitative predictions are presently limited to steady state catalyst operation [2]. Because up to 90% of the allowable exhaust emissions are discharged during the pre-light-off period, a considerable amount of effort is currently being directed towards developing a transient model capable of accurately predicting catalyst warm-up processes. The

ultimate aim is to use such models to modify catalyst designs so as to shorten light-off times.

A number of features within existing transient catalyst models have been identified as possible contributory factors to their relatively poor predictive performance. It is increasingly becoming apparent that accurate prediction of the warm-up process is likely to require a three-dimensional catalyst model capable of simulating the interaction between the upstream flow field and the thermofluid processes taking place in the monolith [1]. In addition accurate prediction, using CFD techniques, of the velocity profile across the inlet face of the monolith may also be required.

Present hardware limitations mean that it is impractical to model, in detail, every channel of a monolith simultaneously [3]. Consequently a commonly used alternative for producing a three-dimensional catalyst model is the equivalent continuum approach. Such an approach requires the specification of heat and mass transfer rates within the monolith using Nusselt (Nu) and Sherwood (Sh) numbers. To account for the augmented heat and mass transfer that occurs within the monolith channel entrance region a variety of expressions relating Nu and Sh to the channel Reynolds number (Re), and axial position, have been used. Most of these relationships, however, have been derived from steady state, non-reaction situations. There is, therefore, a degree of doubt over their appropriateness for transient, reacting conditions. It should also be noted that there is a level of uncertainty over the thermal properties of the monolith, particularly with respect to the anisotropic nature of the thermal conductivity.

Probably the major contributory factor to poor transient predictions are the expressions used to calculate the emission species reaction rates. A limited number of pertinent expressions are available in the open literature, and the majority that are available have been derived under steady state conditions. It has been demonstrated that these

expressions are not reliable under the oscillating air-fuel ratio conditions produced by engine management systems [4]. It is also accepted that certain reaction rate expressions are inappropriate during the transient warm-up process.

Although the above factors are generally accepted as likely to be the main sources of error in transient predictions, there is an additional physical process, the condensation and evaporation of moisture, that has attracted little attention. These effects have not previously been included in catalyst models. This paper identifies the impact moisture in exhaust gases has on monolith thermal behaviour, and demonstrates how these effects can be incorporated into an existing catalyst model. The model is then used to indicate the conditions under which condensation-evaporation processes effect light-off predictions.

2 EFFECT OF MOISTURE

Examination of the temperature history of catalysts warming up from cold frequently reveals a temperature plateau lasting up to 60 seconds. The temperatures at which these plateaux occur vary slightly, but are usually in the region of 50 °C to 70 °C. An example of such a plateau is shown in Figure 1 (data supplied by Johnson Matthey plc), which shows the inlet and outlet exhaust gas temperatures of a vehicle mounted ceramic catalyst: the outlet temperature remains at approximately 60 °C for 30 seconds following the increase in engine speed. In contrast the inlet temperature follows a near continuous exponential rise.

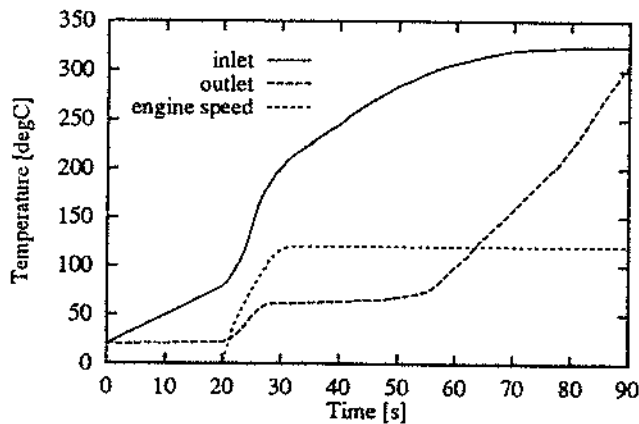


Figure 1 - Catalyst inlet and outlet temperatures following an engine cold start.

The most likely reason for the existence of temperature plateaux in catalyst outlet temperatures is moisture. Confirmation that such effects are not connected with the chemical conversion process is provided by their existence in results from washcoat only catalysts (i.e. no noble metals). It can also be shown that the stoichiometric combustion of a typical fuel produces a mass fraction of moisture in the exhaust gas of approximately 7.6%. If the gas density during the early stages of the warm-up is taken to be 1.2 kg/m³, the specific volume of the moisture will be in the region of 11 m³/kg, which equates to a saturation

temperature of approximately 52 °C. Such a temperature is similar to the plateau temperatures. It thus seems reasonable to suggest that the plateau represents the evaporation of moisture from the washcoat. It should also be realised that if condensation is occurring prior to the onset of the plateau the monolith will experience a slightly accelerated warm-up, through the release of latent heat.

A delay in the warming up of monoliths by as much as 60 seconds would seem to represent a significant handicap to the early onset of light-off. For this reason it was decided to try and model the influence moisture has on catalysts, and test whether they affect the light-off process.

3 MATHEMATICAL REPRESENTATION

To simulate the effects of moisture use has been made of an existing, fully integrated catalyst model, implemented within the PHOENICS commercial CFD code. It is based on an equivalent continuum approach and in addition to including representations of the major thermofluid processes that occur in monoliths it is capable of simulating the interaction between these processes and the upstream flow field. Details of how the model was implemented within PHOENICS, with a demonstration of some of its capabilities, can be found in a previous paper [5].

To allow the effects of moisture to be incorporated into the existing model a simple mathematical representation of the likely condensation-evaporation processes taking place had to be developed that was consistent with the equivalent continuum approach. The resulting moisture model is based on two moisture conservation equations, one for the concentration of moisture within the washcoat and one for the concentration of moisture within the gas phase.

It should be noted that the equations listed below are only applicable within the monolith whereas the original model is capable of simulating the behaviour of exhaust gases outside the monolith. To limit model complexity and reduce the computation time needed for the present work a simplified one-dimensional version of the model was developed. If the moisture model is to be used with the full three-dimensional version, including simulation of the exhaust gas outside the monolith, additional terms have to be included in Equation (1).

The mass fraction of moisture in the gas, c_{gw} , is obtained from a conservation equation of the usual form,

$$\frac{\partial \rho_g c_{gw}}{\partial t} + \frac{\partial \rho_g U c_{gw}}{\partial x} - \frac{\partial}{\partial x} \left(\rho_g D_w \frac{\partial c_{gw}}{\partial x} \right) = S1 \quad (1)$$

The source term $S1$ represents the transfer of moisture between the gas and solid. It is given by,

$$S1 = \rho_g K_{mw} a_v \left(\frac{1}{\rho_g v'_{sw}} - c_{gw} \right) \quad (2)$$

where v'_{sw} is the specific volume of the saturated water vapour at the washcoat surface and K_{mw} is the mass transfer

coefficient for the moisture. The formulation of $S1$ is based on the assumption that the moisture in the washcoat is predominantly in the liquid phase, with a thin layer of saturated vapour adjacent to it. The water and saturated vapour are taken to be in thermal equilibrium with the washcoat. Thus v'_{sw} , which will be a function of the monolith temperature, can be estimated from the thermodynamic properties of steam [6]. To facilitate its calculation within the computational model the algebraic function,

$$v'_{sw} = \exp(1.325 \times 10^{-4} \Theta_s^2 - 0.06 \Theta_s + 5.175) \quad (3)$$

was derived. Note that Θ_s is the temperature of the monolith in °C, and that Equation (3) is only valid for $20 \leq \Theta_s \leq 120$.

The conservation equation for the moisture in the washcoat is,

$$\frac{\partial C_{sw}}{\partial t} = K_{mv} a_v \left(\rho_g c_{gw} - \frac{1}{v'_{sw}} \right) \quad (4)$$

where C_{sw} is the mass of water stored in the washcoat per unit monolith volume.

The last part of the mathematical representation of moisture involves modelling the effect condensation and evaporation have on the temperature of the monolith. When moisture condenses on the washcoat the latent heat of vaporisation is given up to the monolith, which consequently increases in temperature. Conversely, for moisture to evaporate the latent heat of vaporisation must be provided by the monolith, which, if not actually causing a fall in temperature, will prevent the monolith temperature from rising. Both these effects can be achieved with the addition of an extra source term in Equation (9) of reference [5]. It takes the form,

$$S = \frac{C_{sw} - C_{sw}^o}{\Delta t} \frac{h_{fg}}{(1-\alpha)c_{ps}} \quad (5)$$

where h_{fg} is the latent heat of vaporisation and Δt is the duration of the time step. Like v'_{sw} , h_{fg} will vary with the monolith temperature and can be estimated from published data [6]. A very close approximation can be obtained from a linear relationship, however over the temperature range 20 °C to 100 °C acceptable accuracy is achieved by fixing h_{fg} at a constant value of 2370.1 kJ/kg. It should be noted that although Equation (4) can be directly substituted into Equation (5), there by eliminating the moisture concentration in the washcoat from the calculations, it is necessary to solve for C_{sw} to ascertain when all the moisture has been evaporated from the washcoat. Note also that care must be taken to prevent C_{sw} from becoming negative. Details of how the above model was implemented within PHOENICS can be found in [1].

4 MODEL APPRAISAL

It is not possible to assess the reliability of the above mathematical representation of the effects of moisture in isolation. Its reliability has to be tested in conjunction with the underlying original 'dry' catalyst model. As yet a full validation of the 'dry' catalyst model has not been completed; a systematic appraisal is being undertaken at Coventry University. The work presented in [1] and [5], however, indicates that the 'dry' model is capable of at least good qualitative predictions. Even accepting this level of accuracy, the following comparisons between predicted and experimental data assess the reliability of both the 'dry' model and the moisture model together.

To carry out the appraisal use has been made of a set of experimental data collected by Jasper [7], from catalysts connected to an engine test bed. This datum set is particularly useful for model assessment because it contains an extensive listing of boundary conditions, and because the engine was fully warmed before any exhaust gas was passed through the catalyst. The reason for pre-warming the engine, with the catalysts isolated, was so that throughout a test the composition of the gas entering the catalyst section would remain virtually constant. As engines warm-up the composition of the exhaust gas changes significantly. Although pre-warming the engine meant that results from the study are not truly representative of real light-off conditions, the consistent composition of the gas provides a less demanding environment for the reaction rate expressions.

An added attraction of the Jasper [7] study is that it includes warm-up characteristics of washcoat only catalysts (i.e. no noble metals). Data from washcoat only monoliths are particularly useful for establishing how reliable a model is at predicting the heat transfer without the complication of chemical reactions. In view of these comments two cases from [7] were chosen for simulation, a catalyst treated with noble metals, referred to as active, and a washcoat only catalyst. Both consisted of 6 inch long, 3.66 inch diameter ceramic monoliths, with nominal cell densities of 400 cpsi. In addition both had the same assembly geometry, a sketch of which is included as Figure 2.

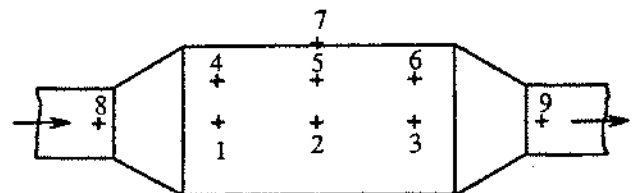


Figure 2 - Catalyst thermocouple locations.

The experimental data collected included nine temperature measurements, six at positions within the monolith, one on the external surface of the can, one in the inlet pipe and one in the outlet pipe. The relative positions of the thermocouples is indicated in Figure 2. The temperatures taken inside the monolith are assumed to be those of the substrate rather than the exhaust gas. Because

only one-dimensional simulations have been carried out, predicted temperatures will be compared with those from thermocouple locations 1, 2 and 3. So that the conversion efficiency of the catalyst could be measured a CO meter was positioned downstream from the catalyst.

4.1 Problem Specification

To limit computational effort only one representative emissions species, CO, was used to drive the chemical reaction part of the model. The exhaust CO and O₂ concentrations were measured, consistently, at 0.5% and 2%, respectively, throughout a series of washcoat only catalyst tests. Consequently these values were taken as the inlet concentrations for the active catalysts. The mass flow rate through the engine was measured at 13.89 g/s. For the one-dimensional simulations included in this work the mass flow was assumed to be uniformly distributed across the monolith. Measurement of the gas temperature as it entered the catalyst showed that it rose exponentially from ambient. To maintain consistency these inlet temperatures were used to specify the inlet boundary conditions.

An initial estimation of K_{mv} was based on the assumption that the Sh would be constant at 3.66. Taking $D_w = 1.66 \times 10^{-4} \text{ m}^2/\text{s}$ gives $K_{mv} = 0.5976 \text{ m/s}$. The properties of the exhaust gas were approximated to be those of dry air. The kinematic viscosity of the gas was made a quadratic function of the temperature, the density being calculated from the ideal gas law. The remaining properties of the exhaust gas, the material properties of the monolith and the other model parameters are those used in reference [5].

4.2 Washcoat Only Predictions

To remove the uncertainty caused by reaction rate expressions and mass transfer coefficients, the initial assessment of the model's performance was restricted to the washcoat only case. As part of this initial stage of investigation a number of model parameters were varied. For example, when a mass transfer coefficient of 0.5976 m/s is used the moisture mass transfer rate is so fast resolution of the condensation-evaporation process requires time steps of the order of 0.01 seconds. To investigate the influence of the mass transfer coefficient, a simulation was run using a K_{mv} value 10 and 100 times smaller. Use of these values allowed time steps of between 0.1 to 0.5 seconds to be used, yet did not significantly affect the behaviour of the gas and monolith temperatures. It was also discovered that the duration of the temperature plateau becomes progressively shorter as the exhaust gas flow rate is increased, and that increasing the mass fraction of water within the exhaust gas raised the temperature at which the plateau occurs.

The duration of the plateau was also extended if the washcoat was given an initial moisture content prior to engine start-up. Data supplied by Johnson Matthey plc indicates that monoliths do absorb moisture when left to stand. The mass of a $1.675 \times 10^{-3} \text{ m}^3$ 400 cpsi ceramic monolith was measured at 0.979 kg immediately after

being cured in an oven. 30 minutes later its mass had increased to 0.989 kg. If the mass increase is due purely to absorption of moisture the initial value of C_{sw} will be 6 kg/m^3 . It is possible that this figure may vary, depending on atmospheric humidity levels. An initial washcoat moisture concentration of 10 kg/m^3 would not seem inconceivable.

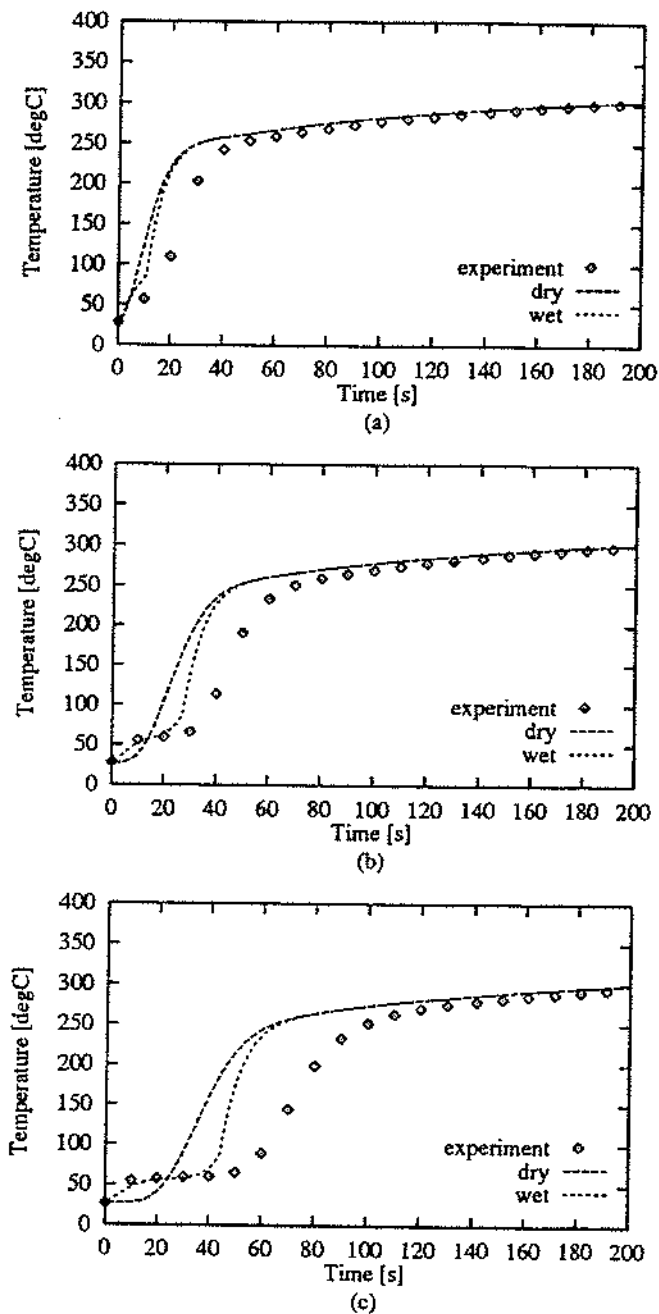


Figure 3 - Predicted (wet and dry curves) and experimental monolith temperatures for the washcoat only catalyst at (a) thermocouple location 1 (b) thermocouple location 2 and (c) thermocouple location 3.

Of these initial studies the simulation that produced the closest agreement with the experimental data used a moisture mass transfer coefficient of 0.005976 m/s, an initial washcoat moisture concentration of 10 kg/m³ and a gas inlet moisture concentration of 0.076 kg/kg. Figure 3 shows the monolith temperatures from this simulation (designated 'wet') at thermocouple locations 1, 2 and 3, together with the experimental values and results from a dry (i.e. moisture not included) simulation.

Note that the temperatures given by the dry simulation are initially too low, yet a few seconds later become too high. Ultimately, however, after 100 seconds very good agreement is achieved with the experimental data. In contrast the wet predictions compare favourably with the experimental data on the initial temperature rise (caused by condensation), the temperature of the plateau, as well as the final solid temperature. There are discrepancies, however, over the duration of the plateau and the rate at which the temperature rises following the plateau, up to the final temperature. The incorrect prediction of the rate of solid temperature rise after the evaporation plateau may be due to the use, within the model, of a monolith specific heat that is too low and/or too high a heat transfer rate. Incorrect prediction of the plateau duration could be explained by the flow rate being too high, or by the initial washcoat moisture concentration being greater than 10 kg/m³.

4.3 Active Catalyst Predictions

Following the relative success of the washcoat only predictions the moisture model was tested under reacting conditions. The majority of the model parameters remained identical to the washcoat only simulations, however to produce better agreement with the experimental data the mass fraction of moisture in the exhaust gas was raised to 12%. Figure 4 compares the monolith temperatures from this simulation with the experimental data at thermocouple locations 1, 2 and 3. Again results from a dry simulation have been included. Close agreement is achieved between the wet predictions and the experimental data, on the initial temperature rise, the plateau temperature and the plateau duration. Unlike the washcoat only simulations, however, agreement on the final temperatures is relatively poor, particularly at thermocouple location 1. It is assumed that this discrepancy results from an over simplification of, and inaccuracies in, the reacting part of the model. Note that not only does the dry model fail to predict the final temperatures accurately, it again fails to correctly describe the thermal behaviour of the catalyst during the early part of the warm-up.

It is also interesting to note that the rate of increase in solid temperature, after the plateau, shown by the experimental data from the active catalyst is greater than the corresponding data from the washcoat only catalyst. In contrast the corresponding results given by the moisture model for the two cases, however, show similar rates of temperature rise. It is assumed that these discrepancies between prediction and experiment again result from weaknesses in the reacting part of the model.

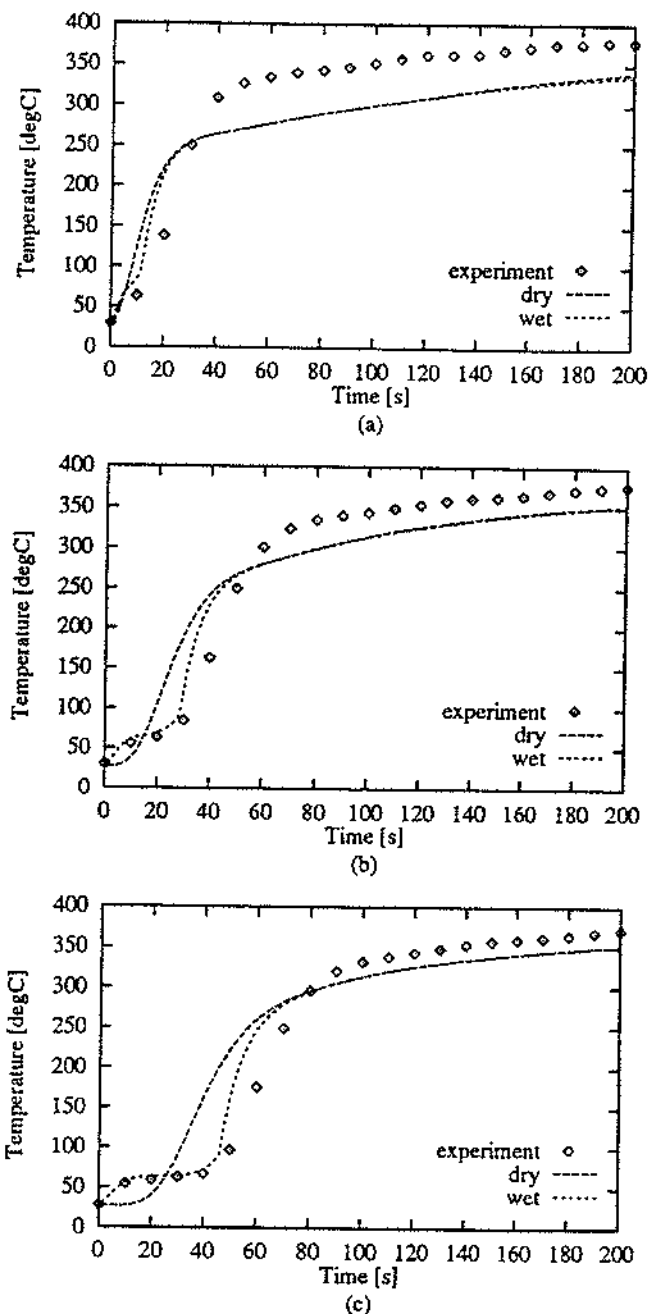


Figure 4 - Predicted (wet and dry curves) and experimental monolith temperatures for the active catalyst at (a) thermocouple location 1 (b) thermocouple location 2 and (c) thermocouple location 3.

Further evidence of the poor performance of the reacting part of the model is obtained from a comparison between the predicted and experimental CO conversion efficiencies, as illustrated in Figure 5. It can be seen that the model fails to accurately predict CO conversion, although the general trends, and time scales, in behaviour are reproduced. The large discrepancy between the final conversion efficiency partly arises, however, from the neglect of external heat loss and the assumption of a

uniform monolith velocity distribution, both of which are usually inherent in a one-dimensional simulation.

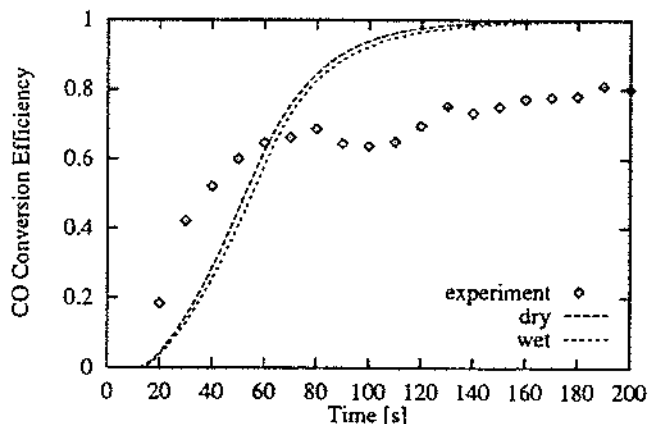


Figure 5 - Predicted (wet and dry curves) and experimental CO conversion efficiencies for the active catalyst.

Accepting the weaknesses in the reacting part of the model, it has been demonstrated that the moisture model reliably reproduces the kind of thermal behaviour experienced in monolith type catalysts during the early stages of their warm-up. There are a number of factors, however, that could influence the accuracy of the moisture model and which might be considered for future refinements. No account is made of the effect the moisture in the washcoat has on the specific heat and thermal conductivity of the solid, and assumptions made about the moisture mass transfer coefficient and latent heat of vaporisation may be in error. Despite these weaknesses it is felt that sufficient accuracy is achieved with both the moisture and reacting parts of the model to justify its use in testing whether the presence of moisture has a significant effect on catalyst light-off.

5 EFFECT ON LIGHT-OFF

It can be seen from the predicted data in Figure 5 that under the conditions investigated above the presence of moisture has little effect on light-off. It is reasoned that this is because the catalyst lights-off towards the front of the monolith. The monolith temperature plots (Figure 4) show that at the monolith front the dry and wet predictions coincide relatively quickly, at a temperature of approximately 250 °C. If significant levels of CO conversion only take place at monolith temperature greater than 250 °C the presence of moisture will make little difference to the onset of light-off. Further along the monolith the temperature at which the wet and dry simulations coincide gradually increases. It is therefore suggested that if the catalyst lights-off towards the rear of the monolith, i.e. the temperature at which significant CO conversion starts to take place (for convenience referred to as the 'ignition' temperature) occurs at the rear, the presence of moisture might have an effect. It is also suggested that if the activity of the monolith were increased, such that the 'ignition' temperature was lowered,

moisture might have a greater effect on catalysts that light-off towards the front.

The occurrence of light-off towards the rear of monoliths has been reported. Thus to test the former of the above suggestions a special set of catalyst conditions were produced that caused the catalyst to light-off towards its rear. These consisted of a reduction in the activity of the monolith at its front, so as to simulate the effect of poisoning, a special reaction rate expression and a gas inlet temperature that rose exponentially from ambient to 250 °C within 30 seconds, but remained thereafter at 250 °C. The reaction rate expression consisted of a rate constant that was a linear function of the monolith temperature between 450 K and 550 K, becoming an exponential function of temperature above 550 K. The exponential part was made to approximate the original CO reaction rate expression.

Using such a reaction rate relationship produces a positive axial temperature gradient that is so shallow the 'ignition' temperature is first reached towards the rear of the monolith. Positive axial temperature gradients (i.e. temperature increases in the direction of the flow) are caused by the slow conversion of emissions species prior to the rapid conversion at, and after, 'ignition'. Catalysts light-off towards the front when the axial gradient is so steep the 'ignition' temperature is reached at the front.

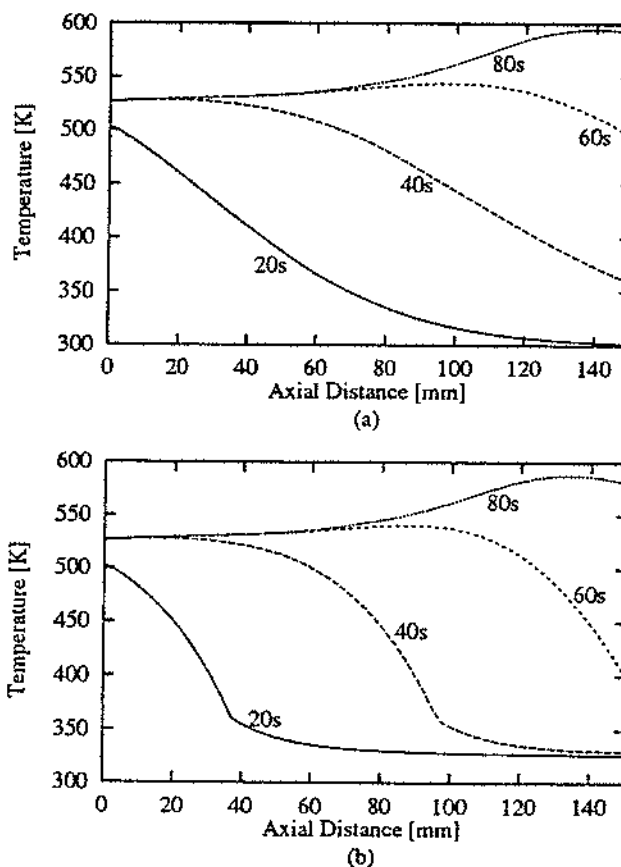


Figure 6 - Evolution of monolith axial temperature distribution for a 'dry' (a) and a 'wet' (b) catalyst.

Figure 6 shows the evolution of the monolith axial temperature profiles for the dry and wet simulations carried

out under the above conditions. Figure 7 shows the accompanying CO conversion efficiencies. It can be seen that the above conditions result in light-off towards the rear, and that the presence of moisture affects the light-off process. If light-off is defined as the point when 50% CO conversion occurs, the presence of moisture delays light-off by approximately 6 seconds. Of more pertinence to emissions regulations is the total mass of CO discharged during the warm-up process. The difference in the predicted masses of CO discharged by a 'wet' and a 'dry' catalyst is represented by the area between the two curves in Figure 7. This difference is only 6% of the predicted mass of CO discharged by the 'dry' catalyst (the area above the 'dry' curve).

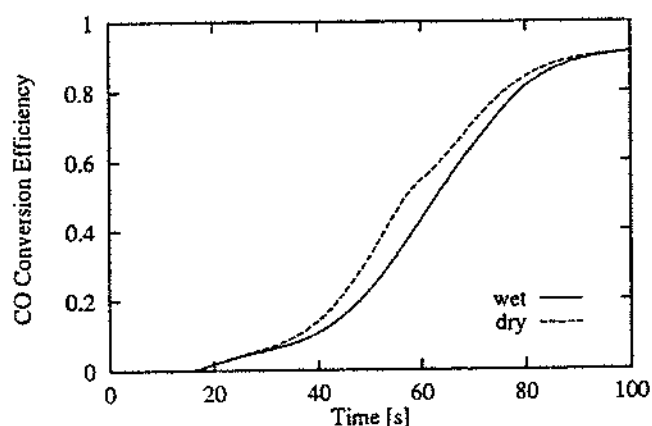


Figure 7 - CO conversion efficiencies for similar 'wet' and 'dry' catalysts.

6 CONCLUDING REMARKS

The moisture present in engine exhaust gases has been identified as responsible for the temperature plateaux that are frequently observed during the early stages of catalyst warm-up. The plateau is due to the evaporation of moisture within the washcoat, which can be present before engine start-up and as a result of condensation from the exhaust gas.

A mathematical representation of the condensation-evaporation processes that occur within monoliths has been developed which is consistent with the equivalent continuum method frequently used for modelling catalytic converters. When combined with such a catalyst model the moisture model is capable of predicting, with very good accuracy, the temperature, and time, at which the evaporation plateaux occur. Not as good, yet reasonable, accuracy was achieved when predicting the duration of the plateaux and the thermal behaviour immediately after the moisture has been evaporated.

Results from the moisture model were then compared with corresponding simulations that did not include the effects of moisture. From these simulations it was possible to show that if a catalyst lights-off at the front of the monolith, neglect of the condensation-evaporation processes has negligible effect on the prediction of

emission species conversion rates. Conversely, if a catalyst lights-off at the rear of the monolith, neglecting the condensation-evaporation processes can produce results that predict light-off several seconds too early. In addition the mass of emissions species discharged during the warm-up process can be under estimated by a figure in the region of 6%. Both these figures, however, are smaller than the level of accuracy that can be expected from the basic, dry, catalyst model. (As part of this work the kind of circumstances that cause catalysts to light-off towards the back of the monolith were commented upon.)

Thus it is suggested that at present greater improvements in the predictive performance of the basic catalyst model can be achieved by refining the reaction kinetics, than can be achieved by the inclusion of moisture effects. However, when these refinements are achieved condensation-evaporation effects will need to be included if accurate predictions of the thermal behaviour during the initial stages of warm-up are required, or if the catalyst is likely to light-off towards its rear.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the financial support given to them by Jaguar Cars Ltd and the EPSRC, that allowed the work reported here to be carried out. We would also like to thank Jaguar Cars Ltd and Johnson Matthey plc (particularly Mr N. Will) for their technical support and guidance.

REFERENCES

- 1 CLARKSON, R.J., A theoretical and experimental study of automotive catalytic converters. *PhD Thesis, Coventry University*, February 1995.
- 2 MONTREUIL, C.N., WILLIAMS, S.C. and ADAMCZYK, A.A., Modelling current generation catalytic converters: laboratory experiments and kinetic parameter optimization - steady state kinetics. *SAE Paper 920096*, 1992.
- 3 JASPER, T.S. BENJAMIN, S.F., GIRGIS, N.S. and CUTTLER, D.H., Computational fluid dynamics and its application to catalyst exhaust systems. *25th ISATA*, June 1992.
- 4 KANEKO, Y., KOBAYASHI, H., KOMAGOME, R., HIRAKO, O. and NAKAYAMA, O. Effect of air-fuel ratio modulations on conversion efficiency of three-way catalysts. *SAE Paper 780607*, 1978.
- 5 CLARKSON, R.J., BENJAMIN, S.F., JASPER, T.S. and GIRGIS, N.S. An integrated computational model for the optimisation of monolith catalytic converters. *1st VTMS Conference, Paper No 931071*, April 1993.

- 6 ROGERS, G.F.C. and MAYHEW, Y.R. Thermodynamic and transport properties of fluids - Third Edition. *Basil Blackwell*, 1980.
- 7 JASPER, T.S. An investigation into parameters affecting catalyst light-off. *MSc Thesis, Southampton University ISVR*, 1988.