Development of computational models for the simulation of the performance of automotive catalytic converters

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ABSTRACT

This paper describes the research work undertaken within the Centre for Automotive Engineering Research and Technology (CAERT) at Coventry University to develop and validate computational models for the simulation of autocatalyst performance. The models predict the flow, heat and mass transfer and chemical kinetics of catalytic converters using as a platform commercially available computational fluid dynamic (CFD) software.

Key-words: Automotive Catalytic Converters, Mathematical Modelling

INTRODUCTION

Optimising the performance of automotive exhaust catalysts represents one of the most challenging tasks facing the design engineer. Converters must effectively reduce emissions whilst not impairing the economy and performance of the engine. At the same time they must be mechanically durable and perform their function effectively over the life of the vehicle.

Stricter emissions requirements have imposed new demands on aftertreatment systems. In particular the need to reduce light-off times has required catalysts to be positioned close to the engine in order that they reach operating temperature in as short a time as possible. This exposes the catalyst to a harsher thermal environment and concern about catalyst durability, both mechanical and functional, is becoming paramount.

Within the industry the development of aftertreatment systems requires many man-years of prototype development and testing. In order to expedite this process design engineers are increasingly turning to simulation methods capable of predicting the performance of these systems. If reliable simulation tools can be developed then prototype designs can be evaluated prior to manufacture and testing. This offers the prospect of selecting and screening the most promising design variants, reducing test programme and development time whilst improving the technical performance of the aftertreatment system.

Hence the development of such simulation tools is an attractive proposition. This paper provides an overview of the research work being undertaken within CAERT to develop and validate such simulation tools. The work has been undertaken in close collaboration with industrial partners and UK government and is in direct response to the needs of the automotive industry.

MODELLING APPROACH

There are several modelling approaches that can be adopted depending on specific user needs. One objective, for example, may be to develop control strategies to minimise emissions throughout a specified vehicle test cycle. In this case it may be considered necessary to simulate the whole engine/reactor system using as a basis one dimensional engine simulation codes. These models will often contain various simple representations of highly complex engine components such as aftertreatment devices and the challenge is to represent these in a physically (and chemically) meaningful way within the one-dimensional code.

At another level models of converters have been developed which accurately describe their three dimensional geometry in some detail. Such models provide valuable information on the spatial and temporal distribution of the three dimensional temperature and flow fields within the converter. These models require as input the gas state immediately upstream of the converter as a function of time and this

is often provided by one-dimensional engine codes or from experimental data. Even these models require, however, a simplified representation of the mass/heat transfer and chemical kinetic processes occurring within each of the 5000 channels typically found in the monolith.

Finally there may be benefits derived from improving the mass transfer processes within the channels of the monolith by, for example, changing the channel shape, washcoat loading etc. In such cases detailed models of individual channels within the monolith may be required. Clearly such a level of detail could not be incorporated into either full engine or three dimensional converter models due to computational resource limitations. However the results from such studies can be used to provide a simplified representation of these processes for inclusion in converter/engine system models.

One of the critical decisions facing the emissions engineer is the design of the converter itself. This has a major influence on the overall engine/system performance. With the trend towards close coupled converters their geometric complexity has increased along with attendant uncertainties regarding the flow and temperature fields within them. Recognising this CAERT has been involved in developing methodologies to simulate such systems for use in the automotive industry. The approach adopted has been to use the solvers of commercially available computational fluid dynamic (CFD) software as a platform into which the physical and chemical kinetic models associated with the reactor are incorporated. In essence submodels of the physical and chemical processes are developed and incorporated into the codes through user defined subroutines. The advantage from a commercial point of view is that the expertise gained in the use of these codes for other applications can be exploited within the company. At the same time general code upgrades can readily be assimilated.

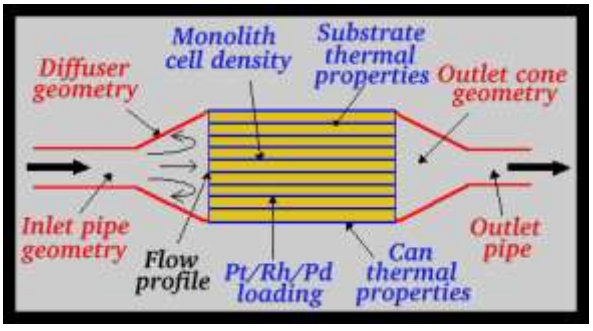

Figure 1 Schematic of a converter.

It is perhaps useful to review the primary processes within the converter so as to ascertain the modelling requirements. Figure 1 shows a schematic of a simple converter. It comprises of an inlet pipe/manifold, diffuser, monolith and outlet cone. The monoliths are coated with an alumina washcoat that supports the noble metals. Monoliths can be either ceramic or metallic and typically comprise of numerous parallel channels with hydraulic diameters of about 1mm. This gives a high surface area upon which reactions take place. Channel geometry is normally either square for ceramic monoliths or sinusoidal in the case of metallic wound structures. Initially the substrate is cold and is subsequently warmed by the hot gases from the engine. The temperature-time history of these inlet gases is a function of the thermal characteristics of the upstream pipework. The exhaust gas on entering the catalyst housing expands through a diffuser into the channels of the substrate. The flow and temperature distribution at the front face of the monolith, which can be highly non-uniform, is a function of the geometry of the diffuser, the resistance of the monolith and the condition of the temperature and flow field (turbulence characteristics, degree of swirl etc.) at the entrance to the diffuser. The latter is largely determined by the complexity of the upstream pipework. On entering the monolith the flow laminarises as the monolith channel Reynolds number is quite low. The substrate is warmed through convective heat transfer from the gas to the monolith surface and then through heat conduction through the monolith structure itself. This of course depends on the thermal properties of the substrate (i.e. thermal mass and conductivity). The gas constituents- HC, CO and NOx are diffused to the washcoat surface and react in the presence of the precious metal catalysts. Initially the reactions are kinetically controlled, as the temperature is low. When the monolith has been sufficiently warmed reactions take place very quickly (light-off) and the conversion process is then mass transfer limited. Exothermic reactions ensure the substrate subsequently heats up quickly and heat transfer then occurs from the substrate back to the exhaust gas. Hence predicting catalyst performance requires a mathematical description of the flow, heat and mass transfer and chemical reactions as a function of both space and time.

Important outputs from a design engineer's perspective are light-off times, steady state emissions, catalyst deactivation and pressure loss. Light-off time is particularly important as prior to this exhaust gases exit the converter untreated. This time must be minimised if future emission regulations are to be achieved. One of the major controlling factors that influences performance is the flow distribution within the converter. Maldistributed flow can have several effects on catalyst performance. It can cause premature degradation of the catalysts in areas of high flow, increased pressure loss, and poor utilisation of the catalyst volume. It is however possible that the concentrated heat flux at the centre of the monolith can reduce light-off times. Whatever the consequences it is

clear that prediction of the flow distribution within the converter is very important.

FLOW MALDISTRIBUTION STUDIES

Figure 2 shows a flow visualisation experiment which illustrates the flow structure upstream of the monolith for a typical underbody converter. It can clearly be seen that the flow separates at the throat of the diffuser and jets across the flow domain. A large recirculation zone is formed between the jet and the diffuser wall. The monolith resistance causes the flow to spread out just before entering the channels. The net effect is that the flow and heat flux is maldistributed within the substrate, with highest velocities and heat flux occurring within the central channels.

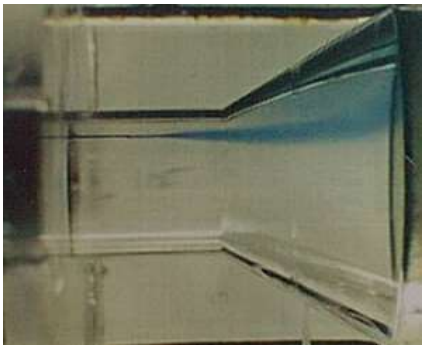

Figure 2. Flow visualisation experiment in a water flow rig.

For close-coupled designs the situation is even more complex. Often the geometry is complicated and the flow is highly pulsating. A schematic of such a converter is shown in figure 3.

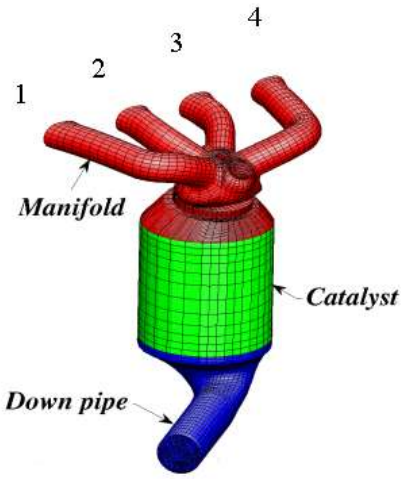

Figure 3 Typical configuration of a close-coupled catalyst.

Figure 4 shows the flow distribution from such a unit as measured at the exit of the monolith on a steady flow rig. Each port was flow tested separately and the velocity distribution was measured at the rear face of the monolith. To facilitate this the outlet cone was removed. Under such conditions the flow distribution appears far from uniform with higher velocities observed towards the periphery. The distribution on a firing engine may, however, vary considerably from this and care must be exercised in deducing too much from such studies. Indeed a programme is currently underway within CAERT to assess the effect of pulsations on converter performance, Benjamin and Roberts (2000).

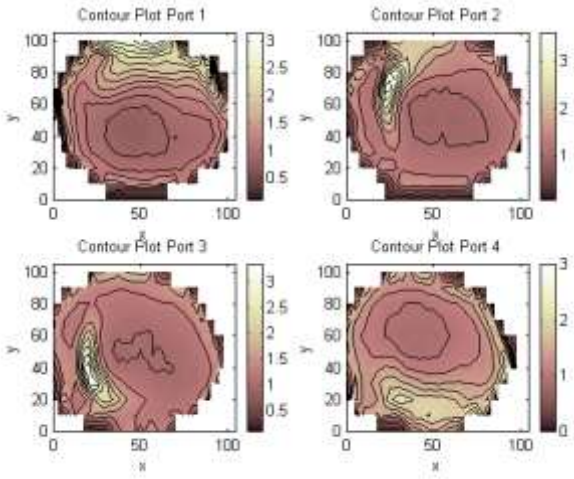

Figure 4. Flow velocity contours (m/s) measured at the exit of a close-coupled converter (x-y location in mm)

Over the last several years a number of programmes has been undertaken to assess the performance of CFD codes in simulating the effect of converter and substrate geometry on flow distribution, Benjamin et al (1996), Clarkson et al (1994), Wollin and Benjamin (1999). The validation programme has focussed on simple axi-symmetric configurations to economise on computational resource. Axi-symmetric systems do however contain the major flow feature of more complex geometries-namely wide-angle diffusers giving rise to maldistributed flow (see figure 2). Studies have been conducted on isothermal and hot air flow rigs under steady and pulsating flow conditions. More recently a programme has been initiated to assess performance for more complex systems on firing engines using laser doppler anemometry.

Figure 5 shows a typical CFD computational grid for an axi-symmetric converter. Resolving the flow domain for each channel of the monolith is impractical and so the monolith is treated as a porous medium with special properties. In other words the flow is resolved only at a macroscopic level within the substrate by

specifying a distributed resistance downstream of the diffuser. The resistance of the substrate is found from isothermal rig studies conducted under well-controlled conditions. Such an approach circumvents the difficulties of modelling each individual channel. Early studies (Benjamin et al (1996)) showed that this approach underpredicted the degree of flow maldistribution. The problem was related to the prescription of the pressure losses at entry to the substrate where, over large sections of the monolith face, the flow approaches obliquely. This can be seen in figure 2. Correcting for this provides much improved predictions as typically shown in figure 6, Haimad (1997).

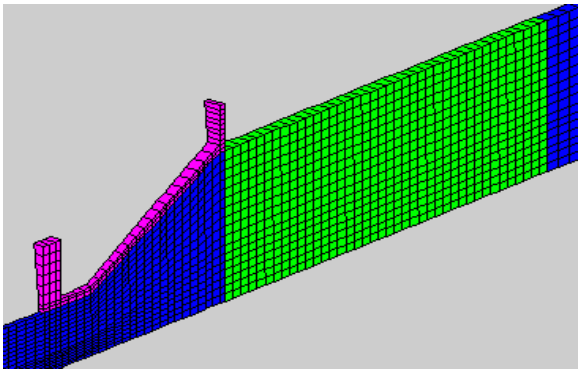

Figure 5 Typical computational grid for isothermal flow simulations.

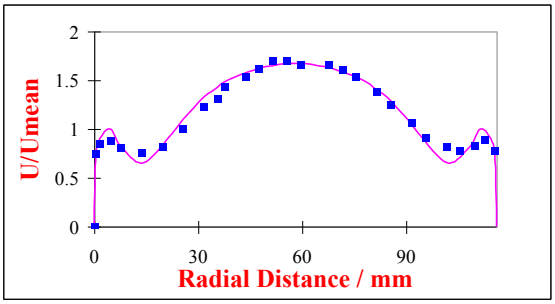

Figure 6 Measured and predicted velocity profiles at the exit of an axi-symmetric converter.

HEAT TRANSFER

Prediction of light-off requires accurate predictions of the flow and heat flux entering the monolith, convective heat transfer from exhaust gas to monolith, and conduction through the monolith structure. For simulation of the full converter it is necessary to treat each of the gas and solid phases of the monolith as a continuum and to specify gas to solid heat transfer coefficients and equivalent conductivities for the monolith. Figure 7 shows a typical computational mesh for the case of a conical diffuser where the fluid and solid phase meshes are illustrated. The heat transfer coefficients (Nusselt numbers) from gas to solid are obtained either from experiments conducted on hot air rigs, Benjamin and Roberts (1998), or from single channel simulations, Day et al (1999, 2000).

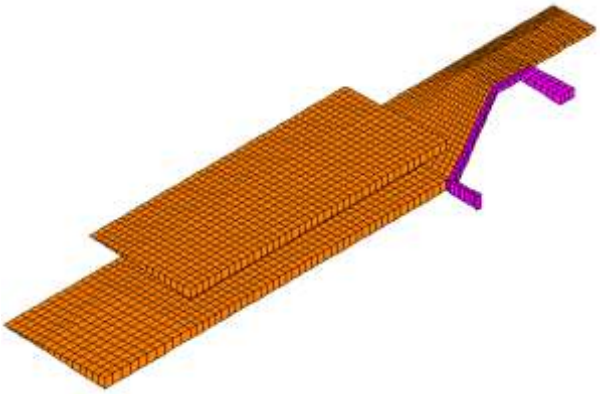

Figure 7 Typical computational mesh for simulating catalyst warm-up.

Figure 8 shows typical measured and predicted temperature profiles along the length of a monolith at different times during a warm up experiment. The converter was fed with a ramp temperature input to simulate catalyst warm up. Good agreement was found over a range of substrates and diffuser geometries, Benjamin and Roberts (1999).

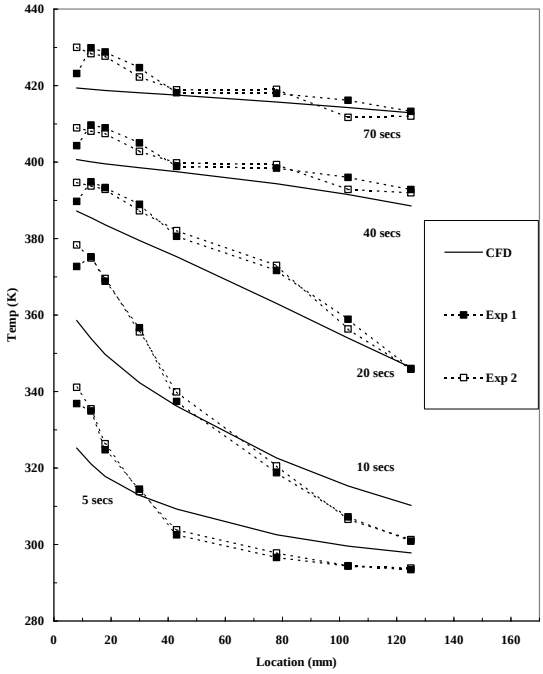

Figure 8 Measured and predicted substrate temperatures along the length of an axi-symmetric converter during warm up, Benjamin and Roberts (1999).

Figure 9 shows the temperature profiles in a metallic substrate obtained from single channel simulations, Day et al (2000). In these simulations the channel is meshed along with the wall and flow and temperature profiles are obtained at each section along the channel. From these it is relatively straightforward to directly obtain Nusselt numbers as a function of distance along the channel as shown in figure 10. These can then be incorporated into a model of the full converter as shown in figure 7.

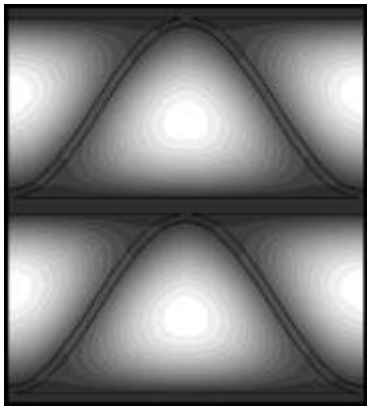

Figure 9 Temperature distribution in sinusoidal channels (equal increments of 0.62K), Day et al (2000).

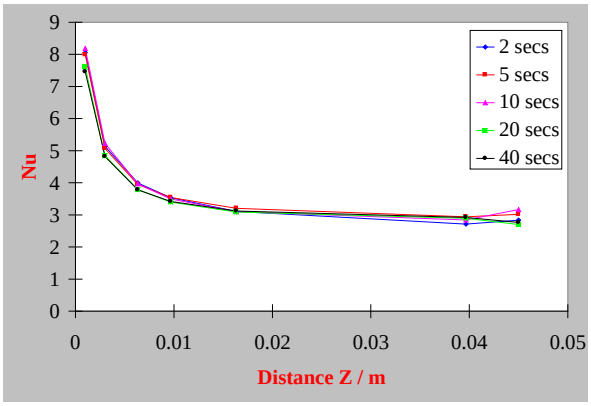

Figure 10 Nusselt Number as a function of distance down a channel during warm up, (Day et al (2000))

LIGHT-OFF

Predicting light-off and emissions requires modelling of the mass transfer processes from the exhaust gas to the washcoat and the chemical kinetics. Single channel simulations can be performed in a manner similar to those described above for heat transfer. Such simulations can also model the diffusion and kinetics throughout the washcoat and so the effect of washcoat loading and precious metal distribution can be investigated. For modelling the full converter the monolith has to be treated as a continuum as described above. Figure 11 shows results from a simulation of light-off for an oxidation catalyst. It shows a case where light-off occurs at approximately 65 seconds from a cold start, Clarkson et al (1993).

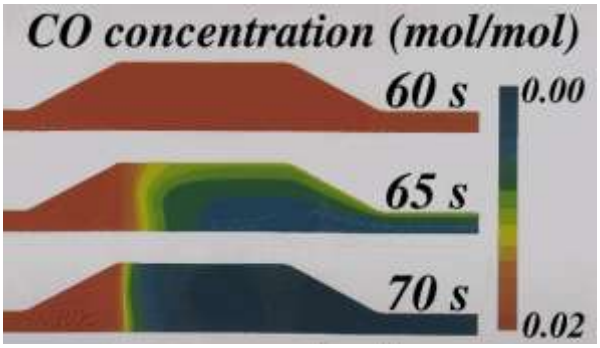

Figure 11 Predicted concentration of CO during light-off.

Figure 12 shows substrate temperatures measured and predicted at a location in a monolith during light off. The results show a temperature plateau occurring early on in the warm up phase, which could not be predicted in the early simulations. This feature is associated with the condensation of the exhaust water vapour on the initially cold monolith and its subsequent evaporation. Much better agreement was achieved once the moisture effect was incorporated into the model as seen in figure 12, Clarkson and Benjamin (1995)

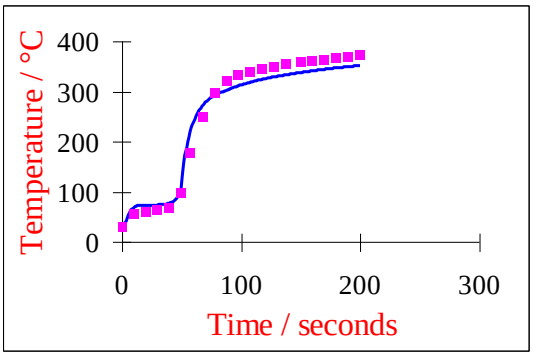

Figure 12 Predicted and measured temperatures in a converter during light-off. Clarkson and Benjamin (1995)

DEACTIVATION MODELLING

It is important that catalysts continue to operate efficiently during the lifetime of the vehicle. As part of the development process converters are subjected to

many hours of endurance testing either on the vehicle or test bed to ensure that performance deterioration is minimised. The factors affecting deactivation are numerous. Thermal deactivation through sintering of precious metals and catalyst poisoning are two of the major mechanisms responsible for decreasing active catalyst area and causing premature ageing. The question arises as to the possibility of developing models to simulate these processes. As an example of this figure 13 shows the results from single channel simulations where the active surface area of the catalysts, Ac (m^2 noble metal (NM)/m^3), has been varied, Manolov (1999). As can be seen this affects the temperature at which the catalyst lights-off and hence emissions. Models are now being developed which can provide functional relationships between Ac and other field variables.

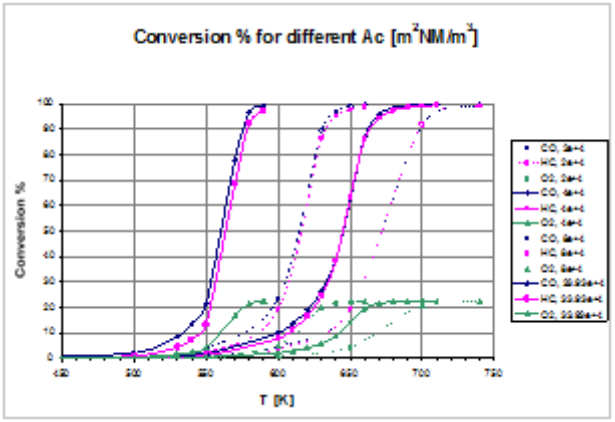

Figure 13 Single channel simulations of ageing. Ac values are shown in the key, Manolov (1999).

CONCLUSION

In conclusion this paper has described research work aimed at developing simulation tools for predicting the performance of automotive exhaust catalytic converters.

Techniques have been developed to simulate and validate the flow, heat and mass transfer and chemical kinetics of converters using, as a platform, the solvers of commercially available computational fluid dynamic software.

Current research is focussing on the effect of modelling and validating conditions with pulsating flow, and catalyst deactivation processes.

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