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Simulating Heat Transfer in Catalyst Substrates with Triangular and Sinusoidal Channels and the Effect of Oblique Inlet Flow

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ABSTRACT

Heat transfer in automotive exhaust catalyst systems with metallic substrates is modeled using a commercial Computational Fluid Dynamics (CFD) code. The substrate channels are modeled by approximating their geometry as both triangular and sinusoidal. The effect of the packing arrangement of adjacent channels is investigated. The effect of the angle of the flow entering ceramic substrate monoliths on the localised heat transfer is also studied and the related implications for catalyst aging and light off deduced.

INTRODUCTION

Catalysts were introduced into automotive exhausts in the early 1970s. Their aim was to reduce emissions to the levels required to meet legislation requirements. Since that time much research has attempted to both identify and quantify the factors that affect both catalyst and engine performance. Modeling of catalyst behavior has become increasingly important. A computational model is highly desirable because it avoids the high costs of testing and design.

In recent years both experimental and predictive work has been carried out in automotive catalyst research at Coventry University (1-3). One approach has been to treat the catalyst as an equivalent continuum so that the fluid dynamics, heat and mass transfer and chemical kinetics associated with the catalyst can be considered as an integrated system. The heat and mass transfer and friction loss are prescribed by assigning appropriate transfer coefficients and pressure loss expressions in accordance with substrate geometry. These transfer coefficients can also be found as a function of axial distance down the monolith channels by a detailed single channel study for a particular geometry. In this way Nusselt number, for example, can be obtained for a particular geometry so that the equivalent continuum model can be made applicable to various channel shapes (4).

With the emergence of CFD and appropriate hardware as readily available tools, an increasing number of mathematical or computational models have been developed for predicting the flow and heat transfer in catalyst systems. The benefits of using such systems include reduced cost and the ability to make rapid modifications to a design.

Both metallic and ceramic monoliths are currently in use as catalyst substrates. Metallic substrates may have a number of advantages over ceramic substrates (5, 6). The thinner walls of metallic substrate channels provide a structure with lower flow resistance but higher surface area to volume ratio. Metallic substrates are less brittle than ceramic and are less likely to crack as a result of thermal stress. Ceramic substrates consist of square cross section channels arranged in a regular pattern. Metallic substrates consist of approximately sinusoidal cross section channels. The corrugated substrate is coil wound into the outer casing of the catalyst system. This leads to an irregular arrangement of adjacent channels.

Shah (7) published flow and heat transfer predictions for isosceles, rounded corner equilateral, sine, rhombic and trapezoidal ducts. These predictions were calculated using a least squares matching technique for fully developed laminar flow and forced convection heat transfer under constant axial heat flux and arbitrary peripheral thermal boundary conditions. Day (8) also looked at the effect of channel shape on substrate performance.

Sherony and Solbrig (9) and Ciofalo et al. (10) both modeled sinusoidal ducts. Their studies were for heat exchangers and so the models were generally concerned with turbulent flow. Their results are applicable to laminar flow where Re is less than 3000. Steady state heat transfer in metallic monoliths consisting of sinusoidal cells has also been studied by Cybulski and Moulijn (11). They considered the sinusoidal cells to be approximated by triangular cells. They assumed negligible pressure loss in each channel and did not allow for hydrodynamic and thermal development at the channel entrance. Nevertheless they obtained reasonable agreement with experimental data.

A theoretical and experimental investigation has already been performed on the heat transfer in a single ceramic substrate channel model under steady flow and on an isolated single metallic channel (present, 4). Relationships between Nusselt number and axial location were proposed which can be used along with the friction factors to describe the heat transfer and monolith resistance in a full catalyst model. These relationships have been found to be largely independent of the major parameters that affect heat transfer for each geometry. The next stage is to give geometric versatility to the full catalyst model by conducting a similar study of metallic substrates. The effect of the orientation and geometric approximation of metallic substrate channels on the heat transfer from the hot exhaust gases to the substrate is investigated in this paper.

The gas entering the substrate channels is assumed to be flowing in an axial direction in the previous models. In practice the flow can enter the channel at angles almost up to 90 degrees to the normal. Whilst this has been shown to significantly affect the prediction of flow distribution (12) the effect on heat transfer is not known. A model of a ceramic substrate channel is used in this paper to investigate what effect the angle of incidence of the flow has on catalyst warm-up.

METALLIC STUDIES

Metallic substrates have a geometry that is close to sinusoidal. It may however be possible to model them as triangular for simplicity. In order to investigate how the geometric approximation affects the predictions of heat transfer in metallic substrate monoliths, both should be used to create two models. The metallic substrate in each case is modeled by means of a representative repeating cell as shown below (figure 1). The arrangement of repetitive cells in the horizontal direction as shown is then regular, whereas in the vertical direction it is irregular. This means that the left and right faces of the cell can be set as symmetry planes, but some other boundary conditions will need to be assigned to the top and bottom faces.

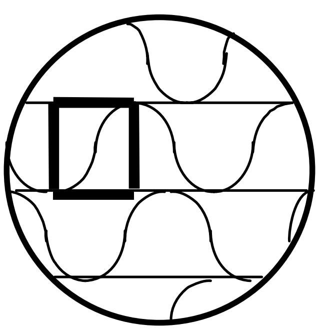

Figure 1. Arrangement of channels in a metallic substrate

The two extreme situations that can occur between two adjacent layers of channels are that the higher layer is in phase with the lower layer or is a mirror image of it. These are demonstrated in figure 2 a) and b) below.

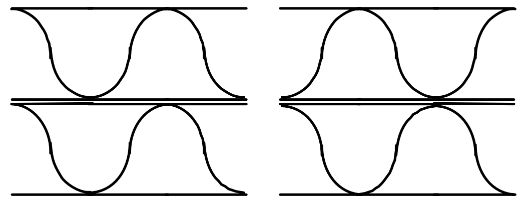

Figure 2. Two arrangements of adjacent layers

MATHEMATICAL REPRESENTATION – The packing arrangement of channels in a metallic monolith, unlike those in a ceramic monolith, varies throughout the cross section due to the manner in which the substrate is wound. In order to assess the effect that the packing has on localised heat transfer, a computational model was created that could predict the heat transfer for different arrangements.

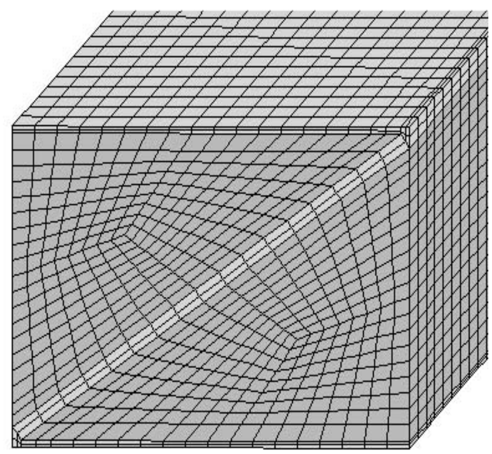

Figure 3. Triangular representative cell model mesh

The CFD code used for the creation of the models was STAR-CD. In conjugate heat transfer, the energy equations for the solid and the fluid are solved simultaneously, with continuity of heat flux held at the solid/fluid interfaces. By assigning different combinations of symmetry planes and cyclic boundaries to the four sides of the repetitive cell used to model the substrate, it is possible to model the two extremes in packing arrangements. Figure 2 a) shows the arrangement modeled by assigning cyclic boundaries to the top and bottom faces, and symmetry planes to the left and right faces. Figure 2 b) shows the arrangement modeled by assigning symmetry planes to all four faces of the representative cell. Figures 3 and 4 show the model mesh of the representative cell using triangular and sinusoidal channels respectively.

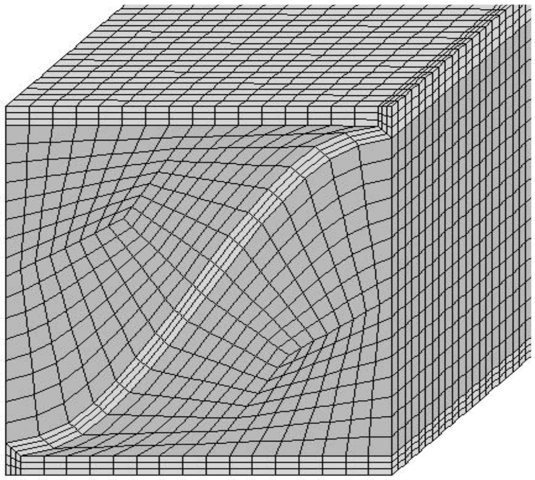

Figure 4. Sinusoidal representative cell model mesh

The other boundaries defined in the models are an inlet plane and an outlet plane. The inlet velocity profile was set to uniform and the magnitude was specified by a constant mass flow rate. For this reason, a portion of fluid upstream of the channel was included in the model. This also allows any effects at the entrance to the monolith to be included in the solution.

The temperature ramp at the inlet was set by empirical equations to match it to the temperature ramp produced by the hot air flow rig on which the experimental investigations (not reported here) are carried out. For this reason the gas properties were set to those of air. Similarly the mass flow rate was set to 6.5 g/s for a 48 mm diameter inlet pipe and the channel dimensions had a characteristic length of about 1 mm.

The assumption made in this single channel approach is that it is possible to neglect radial trends in the full catalyst monolith. The model is therefore a localised multiple channel approximation, where the slight changes of properties between adjacent channels are not taken into account.

One of the user defined programming files in STAR-CD allows for the incorporation of a FORTRAN program which was written to calculate the bulk temperature, wall temperature, heat flux and heat transfer coefficient at any pre-defined number of positions down the channel at whatever time intervals required. Once calculated these are output to separate files for use in an analysis package.

The bulk temperature T_{bulk} was found at each cross section by mass averaging the fluid cells, i.e.

$$T_{bulk} = \frac{\sum T_i . A_{z_i} . \rho_i . w_i}{\dot{m}} \qquad (1)$$

where T_i, A_{zi}, r_i and w_i are the individual cell temperature, cross sectional area, density and axial velocity respectively. The heat flux q can then be found at all solid/fluid interfaces (q_i) and then averaged by surface area.

$$q_i = -\frac{k_{gas}(T_{gas} - T_w)}{d} \qquad (2)$$

$$q = \frac{\sum q_i . A_{x_i}}{A} \qquad (3)$$

where k_{gas} is the conductivity, T_{gas} the temperature of the gas next to the wall and d is the perpendicular distance from the centre of the near-wall gas mesh cell to the wall. Using an average of the wall temperature T_w around the periphery of the cross section the heat transfer coefficient h can be found.

$$h = \frac{q}{(T_{bulk} - \overline{T_w})} \qquad (4)$$

The heat transfer coefficients could then be used to find the Nusselt number Nu as a function of both time and distance down the channel using the hydraulic diameter D_h.

$$Nu = \frac{hD_h}{k} \qquad (5)$$

Once these are known for all the geometric approximations and packing arrangements, they can be transferred to a thin film model for comparison with experimental data.

RESULTS – The Nusselt number as a function of distance down the channel is shown in figure 5 as an average of the values calculated at seven different times. The Nusselt number was found to be largely independent of time, as shown by figure 6 which describes the variation over time for various positions down the channel.

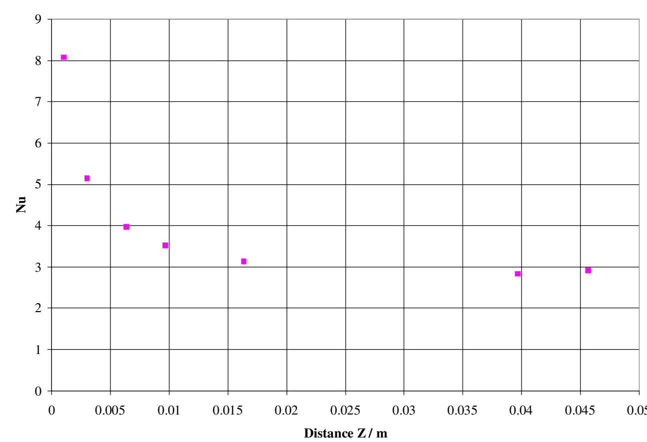

Figure 5. Average heat transfer as a function of distance down triangular channel for a cyclic packing arrangement

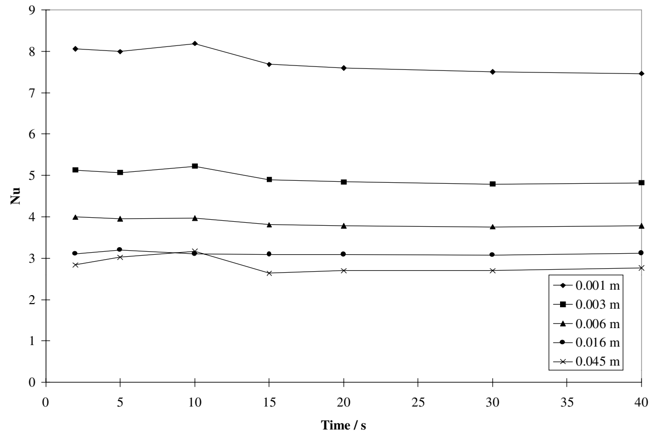

Figure 6. Variation of heat transfer over time at different points down the channel (cyclic)

Figure 7 shows the temperature distribution and the packing arrangement associated with the sinusoidal approximation and the cyclic boundary definitions. Figure 8 shows the same temperature scale in the symmetry plane model.

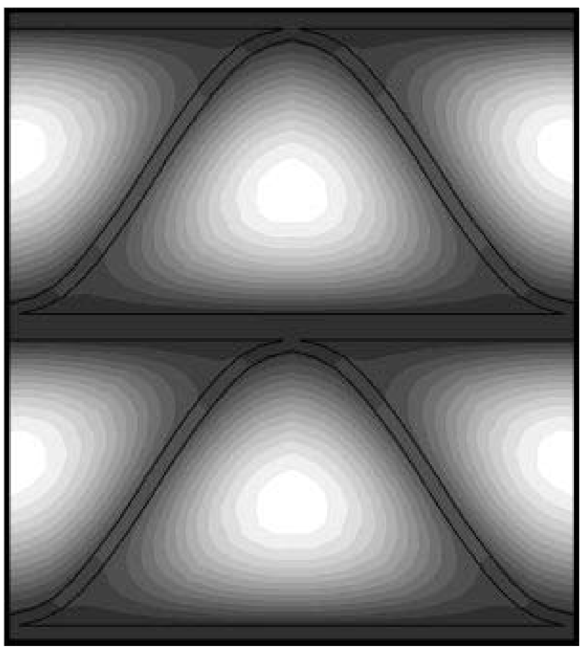

Figure 7. Temperature distribution in the cyclic sinusoidal model (equal increments of 0.62 K)

The effect of the geometric approximation is seen by comparing the temperature of the wall in the middle of the representative cell for the two geometrical approximations and packing arrangements. The wall temperature here will be least affected by the assignment of different boundary conditions to the top and bottom faces.

The temperature of the wall at the centre of the repetitive cell is the same for both packing arrangements for the sinusoidal geometry. There is a small temperature gradient difference however along the wall separating adjacent layers.

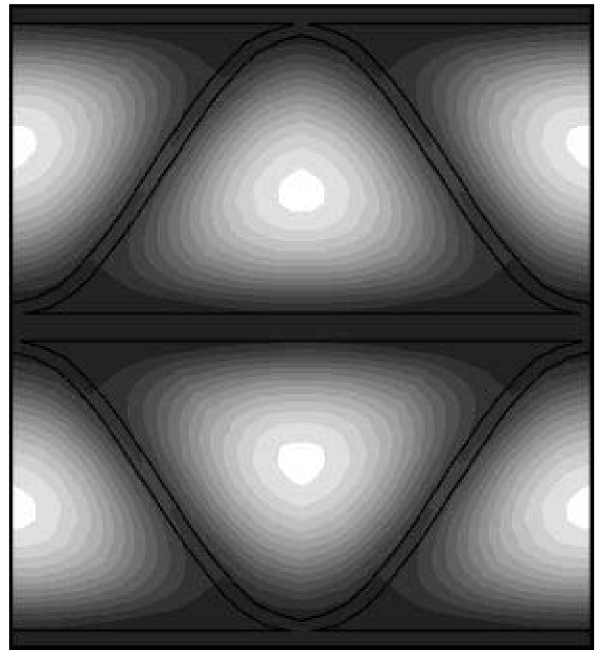

Figure 8. Temperature distribution in the sinusoidal symmetry plane model

The different packing arrangements affected the triangular model to a greater extent than the sinusoidal model (figure 9). This could well be because the sharpness of the top corner in the triangular approximation is reasonable for a single channel but does not properly model the effect of adjacent channels.

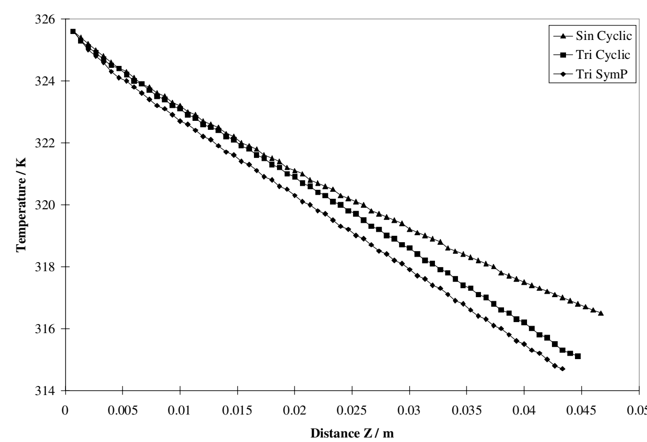

Figure 9. Predicted substrate temperatures at 5 seconds for triangular geometries and cyclic sinusoidal case

The simulation in which all faces of the repetitive cell were set as symmetry planes (figure 2 b)) resulted in reduced warm up of the substrate when compared to the simulation with cyclic boundaries. This could be caused by the proximity of channel corners in the former arrangement. There is little flow in these areas and therefore less effective surface area for heat transfer.

ANGLE OF APPROACH

The air flow into the front face of a catalyst in an automotive exhaust system is not perpendicular in all places. In reality, the angle of incidence varies up to almost 90° to the normal. This angle of incidence will affect the localised heat transfer. In order to investigate how this effect propagates itself, a single ceramic channel model previously developed was extended to allow the angle of attack to be changed.

MATHEMATICAL REPRESENTATION – Due to the loss of one line of symmetry in the flow field a half channel must be modeled, with cyclic boundaries simulating a continuously repeating pattern in the flow field. Two different models were set up. The first model assigned cyclic boundaries to both the fluid and the solid (the situation that would occur in an automotive catalyst) and the second model only assigned cyclic boundaries to the fluid upstream of the channel entrance. This simulates oblique gas flow into a single channel. The heat transfer to both the top surface and to the bottom surface was recorded and compared.

RESULTS – For the first model the gas flow was set up to enter at 0° (for datum), 10°, 30°, 45° and 70° to the normal. The mass flow rate in the channel was kept constant. Results were taken at 2s, 5s, 10s, 15s, 20s, 30s and 40s into the warm-up. The wall temperature around the periphery of the channel was still approximately constant. Separation from the lower surface of the channel was suppressed by the converging flow for angles of incidence of 30° and less. Above that angle there was a separation bubble and recirculation of the flow was clearly visible. Figure 10 shows the entrance region of the channel for 70 degrees incidence angle.

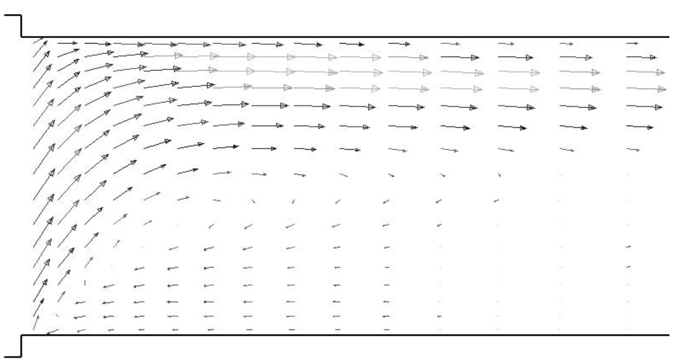

Figure 10. Separation bubble at the channel entrance for 70 degrees incidence.

The two heat flux curves (figure 11) differ in the region of elevated heat transfer (the first 25 mm) associated in previous work with hydrodynamic and thermal boundary layer development (4). The heat transfer to the upper surface is significantly higher than that to the lower surface. After that the heat transfer to the upper and lower surfaces coincide with that found before with axial inlet flow.

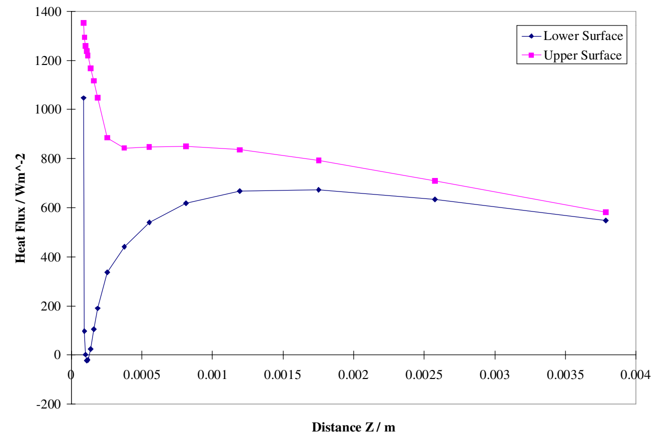

Figure 11. Heat Flux to upper and lower surfaces for 70° incidence

The 'overall' heat transfer to the substrate can be deduced by the effect of the angle of incidence on the substrate wall temperature. Figure 12 shows the wall temperature profile at 30 seconds for each angle.

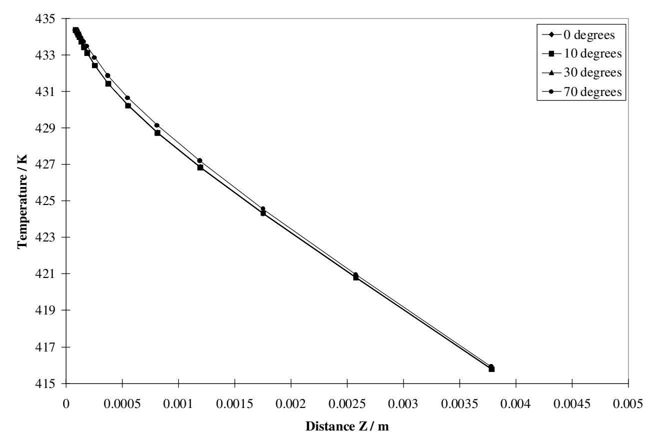

Figure 12. Average wall temperatures after 30 seconds for different angles of incidence

The warm-up of the substrate is seen to be unaffected by the angle of inlet flow incidence for equivalent mass flow down the channel. This is due to the cyclic nature of the model as developed, with the upper surface of one channel transferring heat to the lower surface of the channel above it. The pressure drop across the monolith was found to be affected however as found in previous work (12)

CONCLUSIONS

The packing arrangement of channels in a metallic substrate with a sinusoidal approximation to their geometry has a limited effect on the heat transfer from gas to solid. It is suggested that since models using triangular approximations for the geometry suggest that the packing arrangement does have a significant but small effect, they should be used with caution.

The angle of incidence of the inlet flow to the front face of a monolith has no net effect on the warm-up of the substrate for an equivalent mass flow rate for the cases studied here. It may however influence the mass transfer of species within the washcoat near the front face and the heightened heat transfer on localised parts of the substrate could quicken the process of catalyst aging.

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