Theoretical and experimental investigation of the flow in catalytic converters

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The First IMechE Seminar on:
THE VALIDATION OF COMPUTATIONAL
TECHNIQUES IN VEHICLE DESIGN

Stage One:
COMPUTATIONAL FLUID DYNAMICS (CFD)

18 April 1994

THEORETICAL AND EXPERIMENTAL INVESTIGATION OF THE FLOW IN CATALYTIC CONVERTERS

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ABSTRACT

In response to the increasing use of catalytic converters for meeting exhaust emission regulations, considerable attention is being directed towards improving their performance. One of the main factors affecting catalyst performance is the velocity distribution of the exhaust gases entering the reactor substrate. Thus optimisation of catalyst performance will require a detailed understanding of the flow fields that exist in catalyst assemblies. The cost and time advantages of computational modelling over experimental analysis has meant that CFD is increasingly being utilised as a design tool.

Although validation against experimental data has been claimed by several authors, few systematic validation programmes have been carried out. The present paper includes such a programme for axisymmetric catalyst geometries. Experimental results are compared with CFD predictions, produced using approaches commonly adopted within industry. Significant discrepancies between experimental and predicted results are reported.

INTRODUCTION

Throughout the industrial world automotive emissions regulations are increasingly being adopted. The structure of many of these regulations has meant that, at present, catalytic converters are the only effective solution to the emissions problem. As the regulations become ever more stringent increased attention is being directed towards improving catalyst performance. Additional stimuli have been provided by the desire to reduce component cost and limit the detrimental effect catalysts have on engine performance.

One way of limiting the handicap on engine performance, which results from the elevated back pressures they cause, is to use short catalysts, pressure drop being proportional to catalyst length. However, to ensure sufficient catalyst volume is available for satisfactory conversion of emissions the catalyst cross-sectional area has to be made larger than that of the inlet exhaust pipe. Thus an expansion cone, or diffuser, needs to be used upstream of the catalyst inlet face. Unfortunately lack of packaging space has lead to the use of short, wide angled diffusers. Such diffusers are inefficient at spreading the exhaust gas uniformly across the catalyst, the resulting velocity profiles frequently having a pronounced peak or maximum. Early workers [1,2,3] soon established that these non-uniform velocity profiles have a detrimental effect on conversion efficiency and durability. Thus it is now generally accepted that it is preferable to have a uniform velocity profile across the catalyst face. Improvements in durability and conversion efficiency resulting from more uniform velocity profiles will mean that even shorter catalyst length can be used, which in turn leads to lower costs and back pressures. The problem facing catalyst assembly designers is how to achieve uniform velocity profiles without using long, narrow angled diffusers that have an innate aerodynamic efficiency.

The increases in availability and performance of commercial CFD codes that took place during the 1980's, allied with the improvements made in the power of computer hardware, attracted the attention of catalyst designers. The potential savings on time and cost of computational modelling over prototype testing are considerable. Thus by the 1990's many companies and institutions involved with catalyst design were using CFD codes to study the flow fields in catalyst assemblies [4,5,6]. There is an awareness amongst these CFD users of the technologies weaknesses when predicting the kinds of flow that occur in catalysts; flows featuring streamline curvature and adverse pressure gradients. Despite this however, there are few published results available on the experimental validation of CFD predictions of catalyst flows. Weltens et at. [5] claimed successful comparison for monolith velocity profiles for a small number of geometries, although no comparison was presented for pressure drop data. Thus there is a need for a systematic experimental validation programme to be carried out such that the capabilities of existing CFD technology, for predicting catalyst flow fields, can be evaluated. This paper presents the preliminary results of such a study.

COMPUTATIONAL APPROACH

The flow fields that exist in catalysts are very complex. In addition to the pulsed nature of the exhaust gases, turbulent regimes exist in the inlet and outlet cones, whilst laminar regimes exist in the capillary channels of the monolith bed. It is also possible to show that the mean flow field changes as the catalyst passes through light-off and experiences varying driving conditions. Although the advances made in hardware technology have been considerable, to model all the flow phenomena in detail would still require computer resources beyond the scope of most organisations. Until such resources become available simplified mathematical models have to be employed.

The most obvious mathematical simplification that has to be considered concerns the turbulent flow in the inlet and outlet cones and pipework. For these regions the Reynolds averaged Navier-Stokes equations for incompressible flow are solved, closure being provided by one of a number of available turbulence models. To model the geometric detail of every monolith channel would need a computational mesh of the order of 10^7 cells. Obviously this is not practicable. An alternative is to represent the effect of the flow through the monolith via an equivalent continuum, an approach frequently used to model porous media. To reproduce the effect of the monolith the pressure drop through it must be prescribed using an expression that relates the pressure gradient to the fluid velocities. Neglecting channel entrance effects caused by local separation, decay of turbulence and boundary layer development, the flow through each channel can be taken as having a fully developed laminar profile. The pressure gradient expression for such flow is give by the Hagen-Poiseuille equation,

$$\frac{\partial p}{\partial x} = -\frac{k\,\mu U}{\varepsilon d^2} \qquad \text{EQ(1)}$$

where k is a constant that is a function of the channel cross-sectional shape, x is the flow direction, ε the porosity of the monolith and d the hydraulic diameter of the channels. The justification for neglecting entrance effects is based on the assumption that they contribute little to the pressure drop. This is only true if they exist over short distances and if the monolith is relatively long.

A final simplification that is commonly made is to assume that the flow through the catalyst system is steady, as opposed to pulsating. The arguments against modelling pulsed flow are the extra computational effort and time required and that sufficient information about the performance of a catalyst assembly can be gained from studying their steady flow fields. Whether such a simplification is justified is debatable. It is possible that pulsations make the flow fields significantly different from those that exist under steady flow conditions. However, any debate over whether to simulate pulsations or not is irrelevant if it cannot be demonstrated that the other modelling simplifications, turbulence models and porous media, give satisfactory predictions for steady flow.

A suitable way of demonstrating whether the modelling techniques work is to compare experimental results from simplified catalyst geometries under steady flow conditions against steady flow predictions. To this end a simplified catalyst assembly rig has been built and a range of typical catalyst geometries tested. Simulations of these geometries have been carried out using the commercial CFD code STAR-CD. A selection of turbulence modelling options and numerical schemes have been used, all of which are commonly available within commercial codes. The objective here is to test the sensitivity of predictions to such changes in the modelling approach. The options used for each case are given below. Detailed descriptions can be found in the STAR-CD documentation [7].

EXPERIMENTAL PROGRAMME

The rig was designed so that the flow phenomena known to exist in catalyst assemblies could be studied yet the geometric detail could be kept as simple as possible. Geometric simplicity was required to avoid complicating the flow field with features of secondary importance, such as local separations caused by welds and flow asymmetry caused by pipe curvature. In addition the complexity of the computational grid would be limited. For these reasons an axisymmetric geometry was selected.

One of the main design specifications for the rig was that the boundary conditions for the predictions would be known and could be set using standard CFD techniques. For this reason a sufficient length of straight upstream pipe was provided (50 diameters) to produce a fully developed flow profile at the catalyst inlet. Similarly, the roughness of the internal surfaces was kept as smooth as possible, so that hydraulically smooth boundary walls could be taken. To make velocity measurements easier no outlet cone was attached to the monolith, which consequently exhausts directly to atmosphere. Although the exit cone does influence the velocity distribution across the monolith, Lemme and Givens [2] showed that the effects are small. The flow field produced in the inlet cone is essentially unchanged by the absence of an outlet cone. An added advantage of this approach is that uncertainties over modelling flow in converging sections are avoided. Any discrepancies between predictions and experimental results will only be caused by the inlet geometry and monolith. The outlet boundary condition was taken to be a uniform pressure plane.

The air supply for the rig was taken from an existing compressed air system. The system is fed from two large receiver tanks that are rated up to pressures of 30 bar. The particular limb of the system to which the rig is attached has a "Wizard" control valve between it and the receiver tanks, the purpose of which is to provide a constant downstream pressure from varying upstream pressures. To allow adjustment of the flow rate through the rig a gate valve was positioned downstream from the "Wizard" valve. A viscous flow meter was placed after the gate valve to provide a check that the flow rate was not changing, and allow comparison with the flow rate given by the integrated velocity profiles. A schematic diagram of the rig is included as Figure 1.

Two data sets were selected for comparison with the CFD predictions; the monolith outlet velocity profile and the static pressure drop across the assembly. The main reasons for this being ease of collection, because both sets are pertinent to catalyst performance and because it

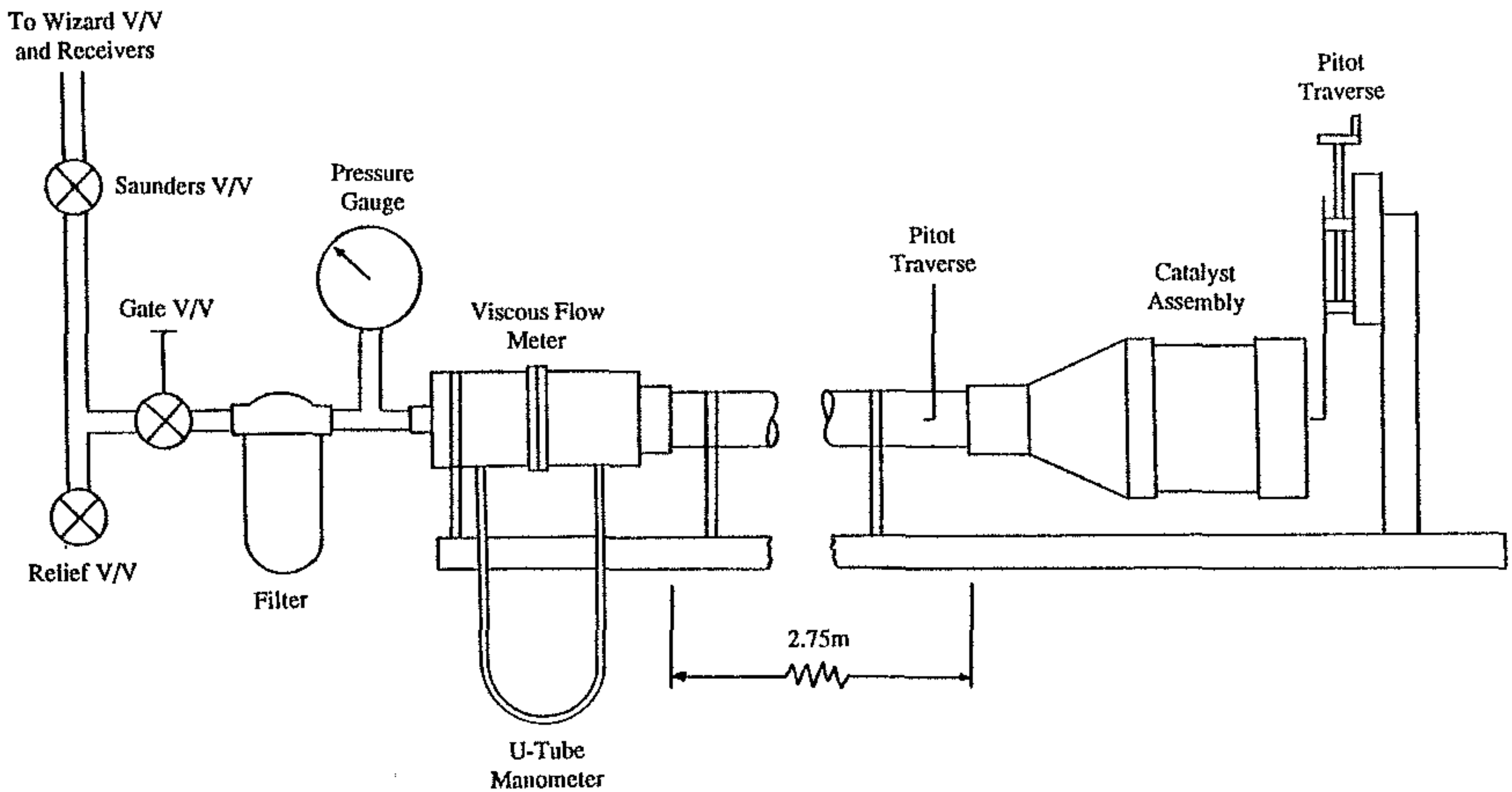

Figure 1 - Schematic of experimental rig

is considered that for reliable prediction satisfactory agreement with both sets of data is required. The inlet static pressure was taken 110 mm upstream from the diffuser throat. The inlet pipe Reynolds numbers (Re) encountered in exhaust flows are typically between 3 000 and 60 000. Will and Bennett [8] have shown that the degree of flow maldistribution increases with Re. Taking the worst flow distribution scenario, experimental data was collected at a Re of 60 000, which equates to a high speed cruise driving condition for a single exhaust, 2 litre engine. Velocities were measured using a pitot tube and accurate inclined manometer. An additional set of velocity profiles was taken 110 mm upstream from the diffuser throat, so that a check of the inlet velocity profile could be made.

The flow emerging from each monolith channel forms a jet, which results in the velocity profile across the back of the monolith consisting of a series of peaks and troughs. 30 mm away from the monolith the peaks and troughs have mixed to such an extent that they cannot be detected above normal turbulent fluctuations. Thus it was decided to measure the monolith exit velocity profile 30 mm from its back face. To prevent entrainment of surrounding air by the jets emerging from the peripheral channels, giving rise to errors, a 30 mm long sleeve was fitted to the rear of the monolith.

The catalyst inlet assemblies chosen for comparison consisted of two axisymmetric diffusers, with wall angles of 40° and 20° respectively, plus correspondingly lengthed 180° expansions, i.e. 37 mm and 84 mm long. Each was fitted with a 6 inch long monolith brick, 4.66 inches in diameter, with a cell density of 400 cpsi. Unwashcoated monoliths were used so that there was a greater degree of certainty over the properties of the porous media.

EXPERIMENTAL AND PREDICTED RESULTS

To limit the number of computational cases and yet still include comparison with a range of geometric variations, it was decided that the various modelling options would be applied to one catalyst geometry, the option giving the most accurate results then being applied to the remaining geometries. The geometry selected for this extended comparison was the 80° diffuser (40° wall angle). The turbulence modelling options used for comparison were,

(i) Standard k-ε model with wall functions, denoted "k-e+wall",

(ii) Renormalization group (RNG) k-ε model with wall functions, denoted "RNG+wall",

(iii) Standard k-ε model with Norris and Reynolds [9] one equation near wall model, denoted "k-e,NR",

(iv) RNG k-ε model with Norris and Reynolds [9] one equation near wall model, denoted "RNG,NR"

Although they do not represent an exhaustive set of turbulence models, they are models that are commonly used. Options (iii) and (iv) are usually referred to as two-layer models.

The full 50 diameter length of inlet pipe was modelled, taking a uniform flow field as the inlet boundary condition. The cross-sectional shape of the monolith channels was taken to be square, giving k = 28.455 in EQ (1). The other values used in EQ (1) were d = 1.12 mm and ε = 77.8%. Initial studies employed an upwind differencing scheme with all four turbulence model options. Two computational meshes were used for the diffuser and the 20 mm of pipe immediately upstream from it; a 45 x 80 cell mesh (mesh 1) for the wall function options and a 30 x 60 cell mesh (mesh 2) for the two-layer options. The latter mesh had an additional 15 cells in the near wall region. All computational meshes were of a "structured" type.

The predicted monolith velocity profiles are all similarly shaped, having their maximum velocity at the centre line and a local maximum adjacent to the monolith periphery (see Figure 2). It is therefore convenient to describe the velocity profiles using one parameter, the ratio of the maximum velocity to the mean velocity, which also acts as an index of flow maldistribution. The maximum/mean velocity ratio and corresponding pressure drops for the cases from the initial study are included in Table 1. The worst and best predictions are compared with the experimental data from the 80° diffuser in Figure 2. These results show that the two-layer approaches give predictions that are closer to the experimental data than the wall function approaches, with the RNG two-layer version being marginally better than standard k-ε version. For this reason the RNG two-layer model was selected for the rest of the study.

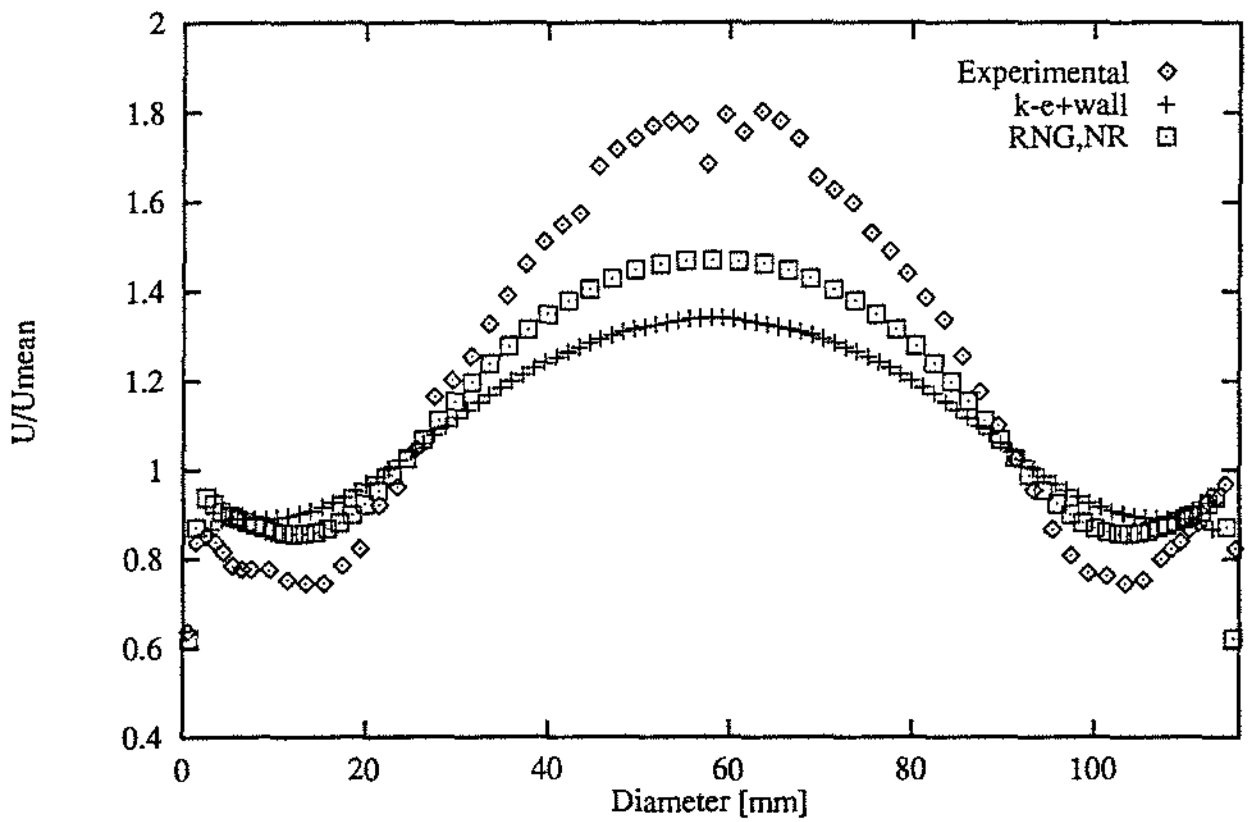

Figure 2 - Best and worst monolith velocity profile predictions for the 80° diffuser using the upwind differencing scheme and meshes 1 and 2

Table 1 - Prediction and experimental data for 80° diffuser.

Mesh	Turbulence Model	Differencing Scheme	$\Delta p/(\rho U^2/2)$ *	U_{max}/U_{mean}
1	k-e+wall	Upwind	1.21	1.34
1	RNG+wall	Upwind	1.20	1.34
2	k-e,NR	Upwind	1.41	1.45
2	RNG,NR	Upwind	1.42	1.47
2	RNG,NR	Hybrid	1.48	1.50
3	RNG,NR	Hybrid	1.47	1.50
4	RNG,NR	Hybrid	1.47	1.50
	Experiment		1.65	~1.78
2+	RNG,NR	Hybrid	0.84+	1.75+

* Pressure drop normalised against mean inlet velocity.
~ Approximate value indicating scattered nature of experimental data.
+ Adjusted Monolith Resistance

The second stage of the study tested for mesh sensitivity. An additional 60 x 120 cell mesh was used with two levels of refinement in the near-wall region, 15 cells (mesh 3) and 30 cells (mesh 4). To reduce numerical errors further a hybrid differencing scheme was used. The results from these simulations have also been included in Table 1. It can be seen that the hybrid differencing scheme improves predictions slightly, however the variation in the results caused by the three meshes is negligible. Note that the hybrid scheme was used for all three meshes. The full velocity profile predicted by option (iv) and the hybrid scheme has been included in Figure 3.

Table 2 - Comparison between experimental and predicted data.

Case		$\Delta p/(\rho U^2/2)$	U_{max}/U_{mean}
80° Diffuser	Experiment	1.65	~1.78
	Prediction	1.47	1.50
37 mm 180° Expansion	Experiment	1.75	~1.78
	Prediction	1.57	1.56
40° Diffuser	Experiment	1.57	~1.65
	Prediction	1.29	1.39
84 mm 180° Expansion	Experiment	1.73	~1.74
	Prediction	1.52	1.52

~ Approximate value indicating scattered nature of experimental data.
Note - All predictions carried out using RNG,NR turbulence model and hybrid differencing scheme.

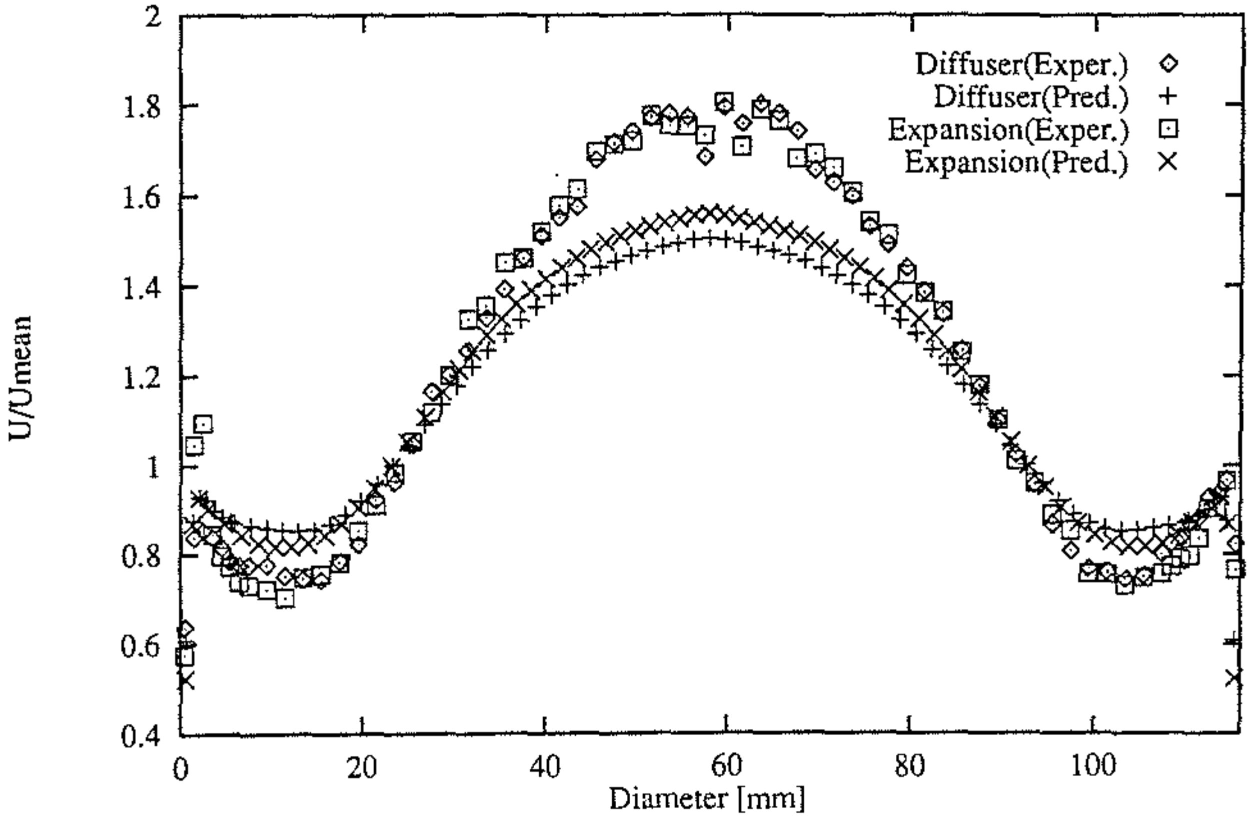

Figure 3 - Experimental and predicted (using RNG,NR and hybrid scheme) monolith velocity profiles for the 80^{o} diffuser and 37 mm 180^{o} expansion

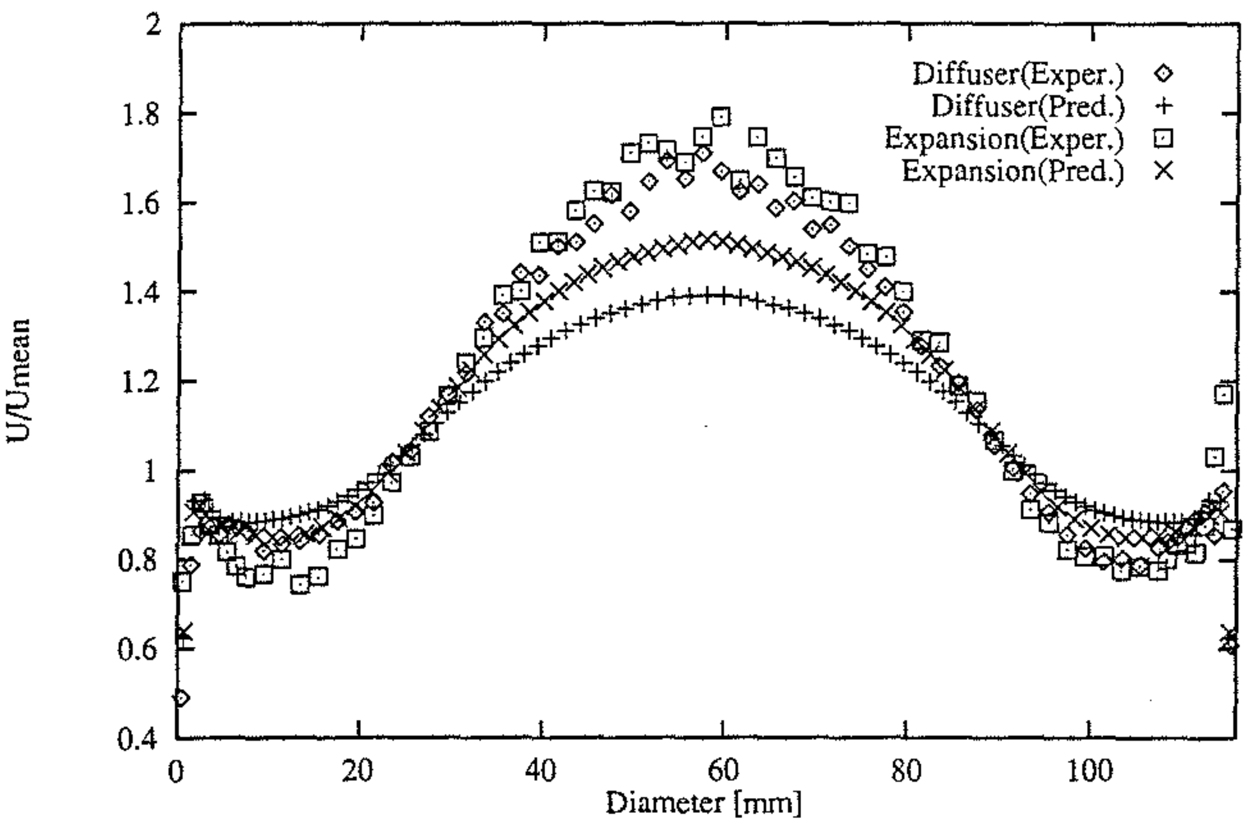

Figure 4 - Experimental and predicted (using RNG,NR and hybrid scheme) monolith velocity profiles for the 40^{o} diffuser and 84 mm 180^{o} expansion

The final part of the study combined the hybrid differencing scheme with the RNG two-layer model to simulated the remaining catalyst geometries. The results from these predictions are presented in Figure 3, Figure 4 and Table 2. It is interesting to note that the experimental velocity profiles for the 80° diffuser and the 37 mm 180° expansion are essentially the same (Figure 3), yet the pressure drop across the latter is slightly greater. The predictions for these two cases do not quite show the same trend, a slight difference in the velocity profiles being calculated. There is a difference between the experimental velocity profiles obtained from the 40° diffuser and 84 mm 180° expansion, a trend that is picked up by the predictions (Figure 4).

DISCUSSION

Despite the improvement in prediction achieved using the RNG two-layer turbulence model and the hybrid differencing scheme there is still considerable difference between the predicted results and the experimental data. The possible causes of this discrepancy are,

(i) numerical errors,

(ii) remaining weaknesses in the turbulence model,

(iii) uncertainty over the expression used to represent the pressure drop through the monolith,

(iv) uncertainty over the accuracy of the experimental data.

The authors believe that the mesh sensitivity test and the use of the hybrid differencing scheme indicate that any remaining numerical errors are unlikely to be significant.

The results obtained from turbulence modelling options (i) and (ii) illustrate the known weaknesses of using wall functions; that the assumption of local equilibrium is not true for severe adverse pressure gradients and separated flows, and that they are unable to represent effects caused by large accelerations resulting from sharp bends (Launder [10]). These problems are exacerbated by the standard k-ε model's tendency to over predict eddy viscosities under adverse pressure gradients (Rodi and Scheuerer [11]) and during streamline curvature (Launder [10]). Both effects lead to the calculated flow remaining attached where experiments indicate otherwise. It is also probable that turbulent mixing in the jet emerging from the inlet pipe is over predicted. Rodi and Scheuerer [11] have shown that the Norris-Reynolds one-equation model can give superior results to the standard k-ε model under adverse pressure gradients. The reason for this probably comes from the prescription of ε using an empirically based algebraic expression. Therefore its use close to the wall not only avoids some of the weaknesses of wall functions but also tends to alleviated some of the problems associated with the standard k-ε model.

The originators of the RNG k-ε model claim that it overcomes many of the weaknesses of existing eddy viscosity methods. Unfortunately the implementation of the RNG k-ε model used in this work is not the complete formulation derived using the RNG method, which allows for resolution of the flow into the laminar sublayer. As has been seen, flow phenomena are strongly influenced by near wall effects, thus any potential improvements in predictions are

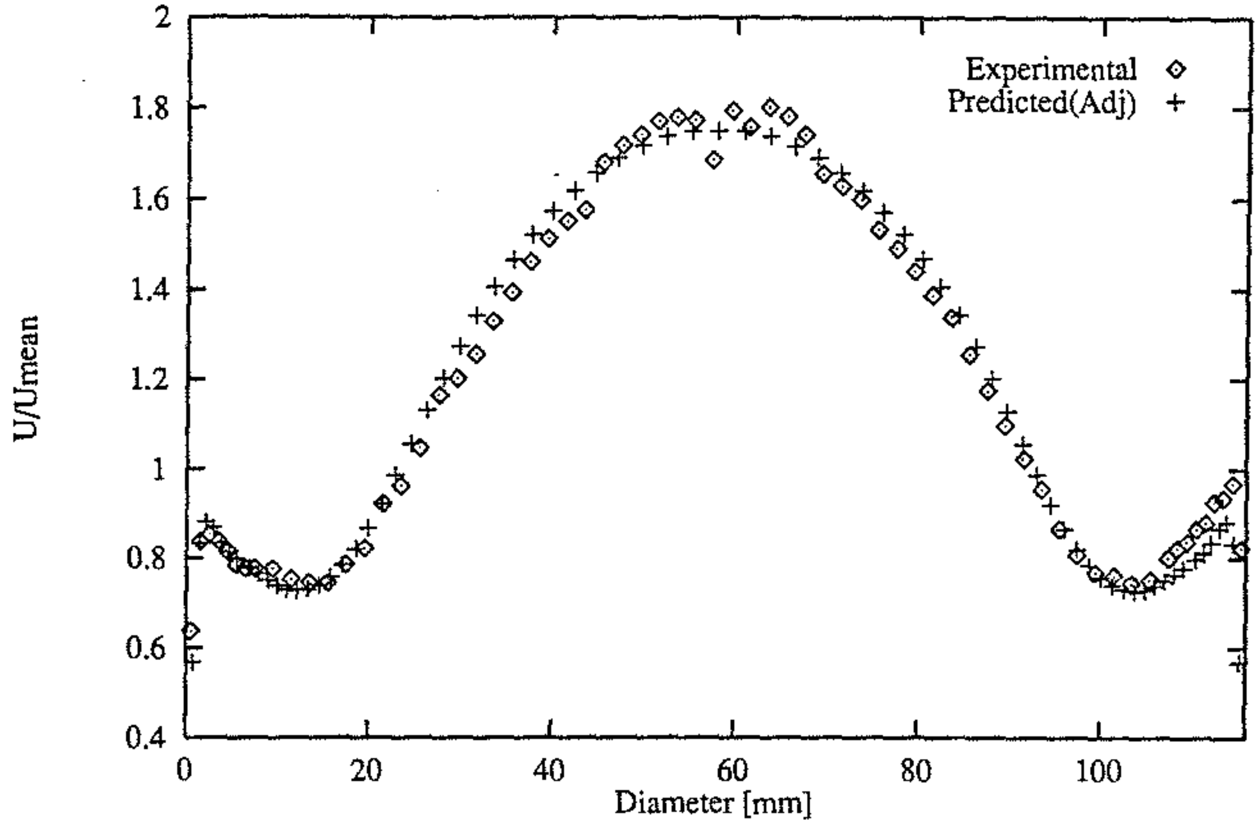

Figure 5 - Experimental and adjusted prediction (monolith resistance reduced to 64.4%) of monolith velocity profile for the 80^{0} diffuser

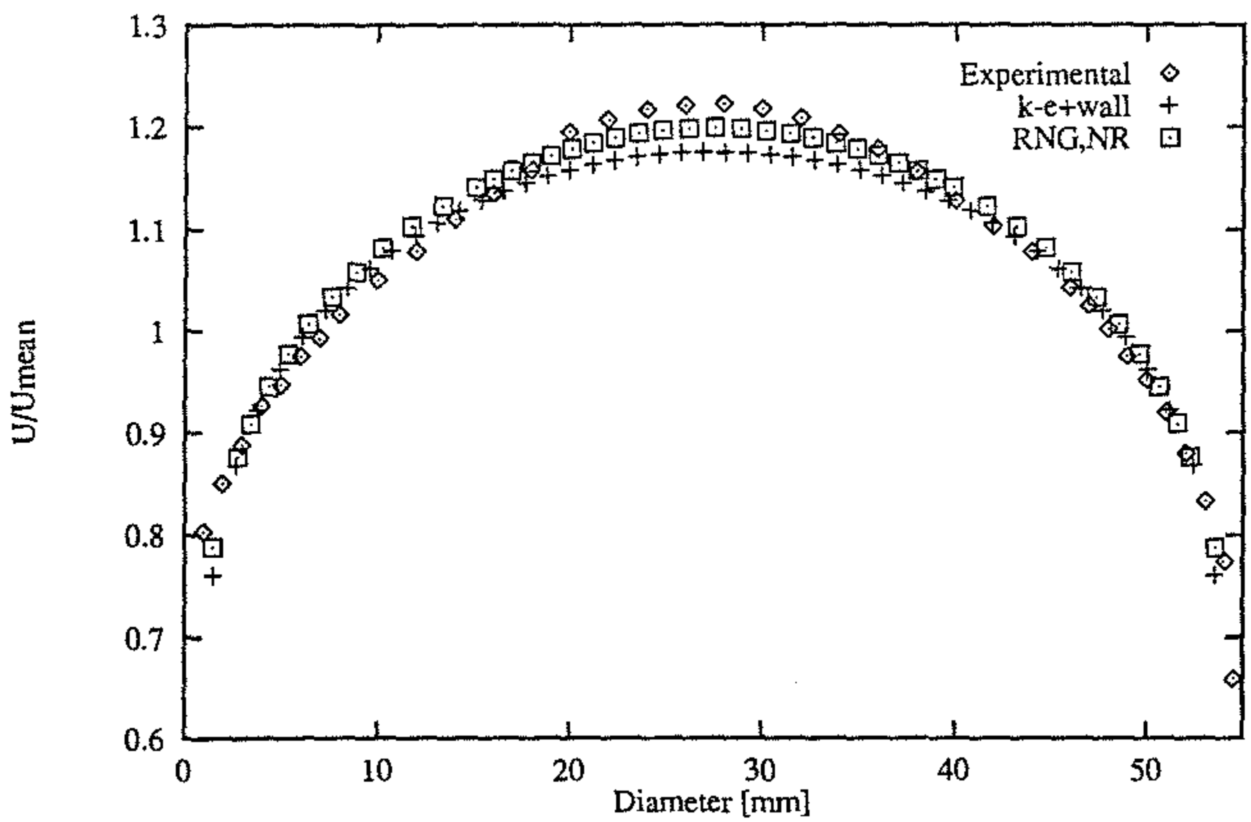

Figure 6 - Experimental and predicted inlet velocity profiles