

# Intra-channel mass and heat-transfer modeling in diesel oxidation catalysts

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## Abstract

We consider the effect of intra-channel mass and heat transfer in modeling the performance of diesel oxidation catalysts. Many modeling studies have assumed that the intra-channel flow is laminar and, thus, heat and mass transfer between the bulk gas and wall are appropriately described using correlations for fully-developed laminar flow. However, recent experimental measurements of CO and hydrocarbon oxidation in diesel exhaust reveal that actual mass-transfer rates can deviate significantly from those predicted by such correlations. In particular, it is apparent that there is a significant dependence of the limiting mass-transfer rate on the channel Reynolds number. Other studies in the literature have revealed similar behavior for heat transfer. We speculate that this Reynolds number dependence results from boundary-layer disturbances associated with washcoat surface roughness and/or porosity. When we apply experimental mass and heat-transfer correlations to multi-channel simulations of a diesel oxidation catalyst, the steady-state conversions differ significantly from those obtained assuming fully-developed laminar flow. These results suggest that assuming fully-developed laminar flow may not always be appropriate.

## INTRODUCTION

With growing concerns about environmental impact, legislated requirements for automobile emissions are becoming ever more stringent. Catalytic monolith reactors are

one of the most widely used components for emissions removal from engine exhaust, but there is still much about these devices that is not well understood. Also, most of the previous modeling work for such reactors has focussed on exhaust from gasoline engines, which operate at near stoichiometric conditions. Pressures for increased fuel economy are encouraging the development of more advanced engines, including spark-ignition engines and diesels that have much leaner exhaust. Unfortunately, it is not possible to directly extrapolate models for stoichiometric reactors to the lean exhaust conditions required for these newer engines.

The focus here is on mass and heat-transfer modeling for oxidation catalysts with typical diesel exhaust feed. Such devices have been used for many years to oxidize carbon monoxide (CO) and hydrocarbons (HC) that remain in diesel exhaust due to an incomplete combustion in the engine. In future aftertreatment systems, it is expected that oxidation reactors will be coupled in series (either upstream and/or downstream) with NO<sub>x</sub> reduction reactors (e.g., NO<sub>x</sub> adsorption or selective catalytic NO<sub>x</sub> reduction reactors). Hence, accurate models for the oxidation catalysts (in the context of diesel exhaust) need to be developed in parallel.

Mathematical models of varying degrees of complexity have been developed for simulating the catalytic converters. Since the Reynolds numbers of flows in monolith channels are typically well below the transition Reynolds numbers, the flows are assumed to be laminar. Hence, mass and heat-transfer coefficients computed us-

ing laminar-flow correlations are often considered to be sufficiently accurate for one-dimensional flow modeling of the channels. As a result, much of the research aimed at developing models for converters (or improving the existing ones) have focused on issues other than heat and mass transfer (kinetics for catalytic surface reactions, adsorption, desorption and storage etc.). Relatively few attempts (e.g. [1, 2, 3, 4, 5]) have been made to study the heat and mass transfer processes or even verify the assumptions underlying the existing models.

The objective of the present study was to evaluate the potential effect of the specific correlations used for estimating intra-channel mass and heat transport in a diesel oxidation reactor under steady-state conditions. In addition, we sought to determine if uneven flow distribution due to reactor entrance recirculation could provide a plausible alternative explanation for observed variations in diffusion-limited mass transport with flow.

## BACKGROUND

Among the most commonly used correlations for modeling heat and mass transfers are the expressions suggested by Hawthorn [6] for computing the axial variation of the Nusselt ( $Nu$ ) and Sherwood numbers ( $Sh$ ) along the axial length of the channels. These expressions are derived using a Graetz series solution for a steady developing concentration (or temperature) boundary layer in a fully-developed laminar velocity field. Similar expressions for various channel cross-sections (e.g. circular, square [3] etc.) have also been derived. In each case, separate expressions have been derived for two possible steady-state boundary conditions : the constant wall condition (for concentration or temperature) and the constant wall flux condition. Since actual boundary conditions at many locations in a catalytic converter often do not strictly coincide with either of these conditions, some reasonable recommendations have been made by Groppi *et al.* [3]. They suggest the use of constant wall flux condition ( $Nu_H$  and  $Sh_H$ ) when the reactions on the wall surface are kinetically controlled (i.e., pre-lightoff conditions) and the use of constant wall temperature condition ( $Nu_T$  and  $Sh_T$ ) once lightoff has occurred.

Additional complications arise when the reactions at the wall are exothermic. The rate of chemical reactions relative to the fluid dynamic processes can be characterized using the Damkohler number,  $Da$ . A  $Da$  dependent expression has often been used (e.g. [3, 5]) for accounting the transition of  $Nu$  between  $Nu_H$  before lightoff to  $Nu_T$  in the post lightoff conditions. While Groppi *et al.* [3] have reported that reasonable predictions can be made using this expression for the transition, Hayes and Kolaczkowski

[5] find that the effective Nusselt number in their multi-dimensional computations deviates significantly from the predictions made using this expression. The disagreement between the two studies can easily be explained as follows.

In the presence of exothermic reactions, not only do the thermal and concentration boundary layers undergo abrupt changes but the velocity field (that convects the transporting species) is also affected by sudden density changes. The expression for the transition of  $Nu$  (across lightoff) does not account for the changes in the velocity field. Since hydrodynamical development was also ignored and the velocity profile was held constant by Groppi *et al.* [3], results that are in line with the expression for transition have been obtained. Hayes and Kolaczkowski [5], however, included the effects of heat release on the velocity field and the resulting changes in the thermal boundary layer (and the heat transfer). Hence the heat transfer predictions using the expression for  $Nu$  transition did not match their multi-dimensional predictions.

The study by Hayes and Kolaczkowski [5] also notes the need to include the effects of evolving velocity field rather than assume a fully developed velocity field everywhere. Such effects would be noticeable at the entrance of the channels and locations where exothermic reactions are intense. The effect of hydrodynamic entry length is perhaps more easily handled since it is characterized in terms of Reynolds number, which is already present in the thermal entry length correction. The effects of chemical reactions are more complicated since, in addition to the reaction rate (quantified using  $Da$ ), the exothermicity (reaction rate weighted sum of the heats of reactions) also needs to be considered. Therefore, any corrections to the heat and mass transfer models to account for the effects of surface reactions based on  $Da$  alone would be specific to the conditions used in a particular study and are not generally applicable.

It is worth noting at this point that most heat and mass transfer studies, including those discussed above [3, 4, 5], have attempted to gauge the accuracy of simplified correlations by comparing their predictions against those obtained from multi-dimensional numerical simulations of channel flows. Though it has been argued in these studies that correlations have to be modified to account for entrance and reaction effects, such modifications seem to have little or no substantial impact on the quantitative predictability of reactor models while simulating real converters. In fact, it has been argued [7, 8, 9, 10] that use of constant  $Sh$  and  $Nu$  produce nearly similar results to those obtained using modifications to the laminar correlations suggested by the above studies [3, 4, 5]. Hence,

constant values of  $Sh$  and  $Nu$  based on the assumption of fully developed, steady state, laminar flow everywhere in the channel were considered sufficient in many of the recent modeling studies (e.g., [7, 8, 9, 10]). The differences between the predictions and experiments were attributed to processes other than heat and mass transfer.

$Nu$  and  $Sh$  have shown a great degree of variability even under similar circumstances. While this has sometimes been attributed to errors in experimentation and analysis [8], there seem to be clear, irrefutable examples of Reynolds number dependences for  $Nu$  and  $Sh$  [11, 12, 13]. The heat transfer studies using microchannels have also revealed strong  $Re$  dependence of  $Nu$  [14, 15, 16, 17].  $Nu$  in most of these studies was found to scale as  $Re^{0.62}$ . When such dependencies have been observed, most authors have attributed the behavior to the roughness effects. Recent experimental measurements of CO and HC oxidation rates in a diesel oxidation catalyst also reveal a similar dependence [18]. However, only two model studies [19, 13] have proposed (or used) expressions for  $Nu$  or  $Sh$  (or both) that include significant  $Re$  effects.

Interestingly, many studies of mass and heat transfer in packed-bed reactors have repeatedly shown strong dependencies of  $Sh$  and  $Nu$  on flow [20, 21, 22, 23, 24, 25, 26, 27, 28]. Correlations of the form  $Nu \sim Re^n$  with  $n$  ranging from 0.4 to 0.92 have been reported for packed beds. In most cases, however,  $n$  was found to be close to 0.6 (e.g., [20, 23, 24, 28]) thereby producing a scaling law for heat transfer that is quite similar to one obtained for micro-channel systems. The  $Re$  dependence in packed beds has been traditionally explained as the result of turbulence generated in the irregular interstitial channels that form between the bed particles. Even though the flow geometry in monolith channels is more structured, the minor irregularities and the roughness of the channel surfaces seem to create flow disturbances that result in strong  $Re$  dependencies of  $Nu$  similar to those in highly unstructured flows like in packed beds.

A possible alternative explanation for a global dependence of  $Nu$  and  $Sh$  on  $Re$  in monolith channels could be the uneven distribution of flow caused by entrance recirculation upstream from the monolith. Uneven flow distribution in the monolith would cause some channels to experience higher residence times and some lower residence times, as well as potentially alter the temperature profile. Because reported values for  $Nu$  and  $Sh$  are typically averaged over the whole multi-channel reactor, the effects of flow redistribution might be incorrectly attributed to a direct dependence of mass and heat transport in each channel on the average channel flow. Multi-channel sim-

ulations have indeed shown marked unevenness in flow among the monolith channels [29, 30, 31, 9, 10, 32]. This non-uniformity also often varies with  $Re$ .

For this study, we addressed the question of whether intra-channel or uneven flow distribution effects was more important by doing simulations of alternative scenarios and comparing the predicted trends with experimental data. Specifically, we compared predicted CO and HC conversions in a diesel oxidation catalyst for a range of cases that included different contributions from inlet zone recirculation and intra-channel mass and heat transport.

## SIMULATION STUDIES

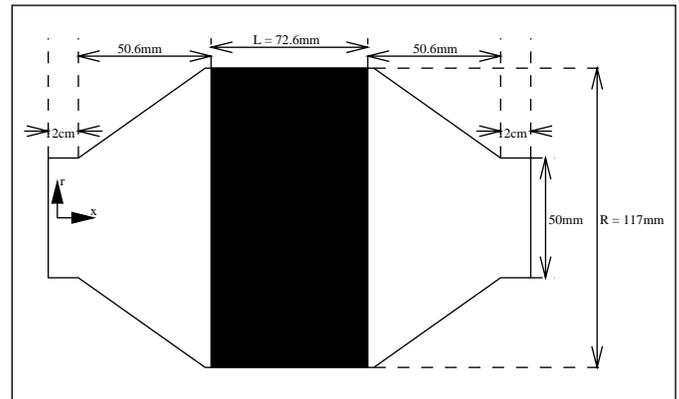


Figure 1: Geometry of the converter

The geometry of the converter used in the simulations is shown in Figure 1. The properties of the monolith reactor are presented in Table 1. The exhaust gas was assumed to consist of 340ppm of CO, 154ppm of HC (assumed to be propene here), 2.32% water, 2.68% carbon-dioxide and 16.54% oxygen. The rest was assumed to be nitrogen. Since the primary simulation objective was to observe oxidation of CO and HC, all NOx related reactions were ignored.

quantity	value
length	0.073 m
diameter	0.0117 m
$\epsilon$	0.7435
cell density	620000 m <sup>-2</sup>
hydraulic diameter	1.095 mm
substrate density	2630 kg.m <sup>-3</sup>
conductivity	1.675 W.m <sup>-1</sup> .K <sup>-1</sup>

Table 1: Monolith specifications

An initial temperature of 300 K was assumed for the monolith and exhaust gas. To induce lightoff, the exhaust

gas temperature was steadily increased to 573 K over a period on 1 second and then held constant. Though the experimental measurements were available only at steady states, unsteady equations are integrated in time until a steady state is reached. The lightoff transients following a cold start predicted by the multi-channel model are used to evaluate the performance of an equivalent one-dimensional reactor model. The simulations were conducted using five different space velocities (definition based on the volume of the monolith channels) ranging from  $16.5s^{-1}$  to  $133.1s^{-1}$ .

Other operating parameters were based on recent experiments for which oxidation rate measurements were available [18]. Briefly, these experiments involved direct measurements of steady-state CO and HC oxidation conversions for the standard OEM-supplied oxidation catalyst on a Volkswagen 1.9 L turbo direct injection (TDI) diesel engine. The measurements were made with the engine mounted on a test stand and connected to an eddy current dynamometer for controlling speed and load. The catalyst was mounted approximately 1.5 m downstream of the exhaust manifold. A fraction of the exhaust stream was bypassed around the catalyst in order to control the exhaust flow rate through the catalyst. Volumetric flow rate through the catalyst was varied over a range corresponding to space velocities from 15,000 to 100,000  $hr^{-1}$  (based on the shell volume and exhaust at standard temperature and pressure). Catalyst inlet temperature was controlled with engine load and varied from 373 to 623 K. Steady state emissions measurements at the inlet and outlet of the catalyst included CO and total hydrocarbons.

Experimental estimates of the limiting mass-transfer rates were determined from the oxidation reactor measurements by observing the asymptotic conversions of CO and HC as the reactor operating temperature was increased. It is well known that as temperature is increased, mass transfer in the gas layer adjacent to the wall becomes the rate limiting step. As described later, the value for the mass-transfer coefficient can be estimated from the observed oxidation reaction rate as this asymptote is approached.

As in the experiments, the simulated monolith was cylindrical with a diameter of 11.7 cm and a length slightly over 7.2 cm. The entrance and exit zones of the experimental reactor were not strictly radially symmetric, but for simulation purposes symmetry was assumed (Figure 1). We believe the symmetry assumption is reasonable because the cone expansion ratios are the same and hence the associated recirculation cells should still scale similarly with inlet flow (i.e.,  $Re$ ).

The flow solver used here is similar to one used in an earlier computational study [33]. The only differences are that the current solver uses axi-symmetric flow equations and a staggered mesh instead of the two-dimensional equations and a non-staggered mesh that were used previously. One-dimensional transport equations are used to model the flow of mass, momentum and energy through each of the channels. Details about the coupling between one-dimensional channel models and the multi-dimensional flow solver have already been explained in the past [33].

Two sets of simulations are conducted in order to explain the experimental observations. In the first set, heat and mass transfer coefficients are obtained using  $Nu$  and  $Sh$  corresponding to developing, laminar steady state flows in ducts (laminar correlations with modifications to include entrance effects). The entrance corrections depend on channel  $Re$  and given the intent of the present study (to explain the  $Re$  dependence of  $Nu$  and  $Sh$ ), it is deemed necessary to include them despite the fact that (as mentioned in an earlier section) their effect on the overall predictions in reactor studies seems minimal [8].

In the second set of simulations, the following expression for  $Sh$  derived from experiments conducted under mass transfer limiting conditions ([18]) is used.

$$Sh = 0.128Re^{0.62} \quad (1)$$

The above scaling law was originally derived for the effective Sherwood number of the reactor in terms of an average channel Reynolds number. This scaling is similar to one obtained for Nusselt numbers in various micro-channel heat transfer studies [14, 15, 16, 17]. Though the Nusselt numbers in question are often the effective Nusselt numbers, the applicability of a similar scaling law in a multitude of different multi-channel heat exchanger designs suggests that the scaling actually applies locally within each channel as well as for whole reactors. The similarity of the  $Nu$  scaling in these studies to the  $Sh$  scaling in catalytic converter experiments suggests an analogy between thermal and chemical scalar boundary layers. So, the local  $Nu$  in the simulations is also determined using a scaling law similar to one in equation(1).

The scaling law in equation(1) was derived under mass transfer limiting, steady state conditions when the surface concentrations of reactants are near zero and wall temperature is constant. However, its use for modeling mass transfer during pre-lightoff conditions can partly be justified since kinetics rather than mass transfer rates control the converter operation. So, any error in mass transfer

modeling at this stage would be negligible. This, however, is not true for the heat transfer modeling. The lightoff times are determined mainly by the heat transfer rates and any error in modeling heat transfer would be reflected in terms of error in prediction of lightoff times. Given that cold start emissions constitute a significant portion of the total emissions from automobiles, lightoff times need to be minimized to the extent possible. Accuracy of the heat transfer models in predicting the heating of the catalyst by the exhaust is, therefore, critical. The need for accuracy is more acute under diesel conditions since the exhaust gas temperatures are usually much lower than in gasoline exhaust. The validity of this scaling law for  $Nu(\sim Re^{0.62})$  during the transient heat up phase following a cold start (pre-lightoff conditions) still needs to be confirmed experimentally.

The following kinetic rate expressions for CO and HC oxidation were also obtained from the same experimental diesel oxidation catalyst study [18].

$$R_{CO} = 4.74 \times 10^{18} \exp \left[ -\frac{16000}{T} \right] \quad (2)$$

$$R_{HC} = 5.41 \times 10^{13} \exp \left[ -\frac{11000}{T} \right] \quad (3)$$

These kinetic expressions were derived using steady state data. For the lack of any further information, they are assumed to be valid also during under transient conditions. It is also worth noting that these global kinetics do have important differences from those that have often been used for oxidation reactions while modeling gasoline exhaust after treatment in three-way catalytic converters (e.g., [7, 8, 9]).

## RESULTS AND DISCUSSIONS

The steady-state mass flow distributions at the inlet face of the monolith for various flow rates are shown in Figure 2. The non-uniformity steadily increases with increasing flow rate (and average channel Reynolds number).

The mass-flow distribution is determined by the flow expansion in the inlet cone and the frictional pressure drops across each of the channels. As the flow expands in the inlet section, it can separate and create a recirculation zone. The recirculatory patterns can lead to high axial velocities around the centerline and lower axial velocities at the outer edges. Hence, the channels around the centerline have high velocities compared to those closer to the outer edge of the converter. The frictional pressure drop

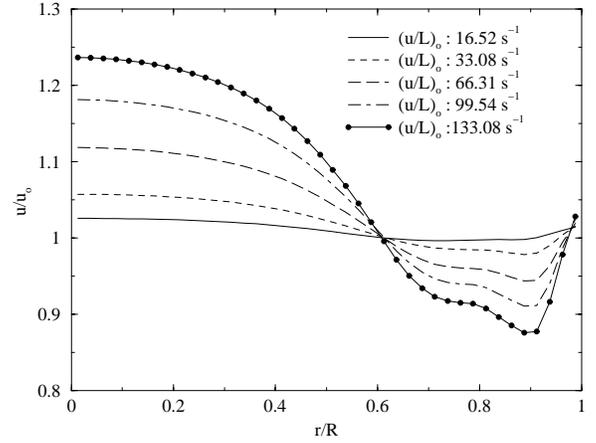


Figure 2: Flow distribution at various space velocities

in monolith channels can be quite high because of the low hydraulic diameters of the channels. The pressure drop increases rapidly with increasing velocity in each of the channels. Since the channels with higher flow rates offer higher frictional resistance than those with lower flow rates, the pressure field would try to redirect more fluid into channels with lower flow rates (i.e., fluid tends to flow through paths of lesser resistance by virtue of the pressure field). Thus, the frictional effects tend to make the flow distribution among the channels uniform. The flow distribution seen at the inlet face of the monolith is therefore determined by two factors: recirculation pattern and frictional pressure drop distribution across the monolith. Recirculation tends to make the distribution non-uniform while pressure drop does the opposite. Both the strength of the recirculation pattern and the frictional effects (i.e., tendency to make the flow uniform) increase with increasing overall flow rate (or equivalently the average channel flow rate or channel  $Re$ ). But, as seen from Figure 2, the effects of recirculation grow faster and thus the flow distribution becomes more non-uniform with increasing net flow rate.

Since the model for the frictional pressure drop is the same in both sets of simulations (one with laminar correlations for heat and mass transfer and the other with corresponding experimental correlations), the flow distributions at a given net flow rate are identical in both sets. Any differences in conversion efficiency solely result from the differences in heat and mass transfer models. The effective  $Sh$  for the multi-channel system would depend on the flow distribution (in addition to the local  $Sh$  in each channel) and since the flow distribution varies significantly with  $Re$ , one can expect some  $Re$  of the effective Sherwood number even if the local Sherwood numbers are independent of  $Re$ . The effective  $Sh$  are extracted from the data

using an equivalent single channel reactor model. The following equations for mass conservation in the channel and on the surface are used in this model.

$$\epsilon u \frac{\partial C_g}{\partial x} = KS(C_s - C_g) \quad (4)$$

$$KS(C_g - C_s) = RC_s C_{s,O_2} \quad (5)$$

All variables in the above set of equations are to be interpreted as cross-sectional averages of corresponding local variables. For steady state and mass-transfer limiting conditions, the conversion efficiency,  $\theta$  is easily obtained in terms of the mass transfer coefficient and the space velocity ( $u/L$ ). Knowing  $\theta$ , the mass transfer coefficient,  $K$  (which is proportional to  $Sh$ ) is easily computed as follows.

$$\theta = 1 - \exp \left[ -\frac{KS L}{\epsilon u} \right] \quad (6)$$

$$K = -\frac{\epsilon u}{S L} \log(1 - \theta) \quad (7)$$

The variation of  $K$  at with average space velocity computed using  $\theta$  from simulations with developing laminar flow correlations is shown in Figure 3. Though the mass transfer coefficients for CO and HC seem to depend on the space velocity (or equivalently the  $Re$  which is proportional to space velocity), the dependencies are not as strong as in the experiments. The weak dependence on  $Re$  could have resulted from the increasing non-uniformity of the flow distribution with  $Re$  or the entrance length correction to the laminar correlations that is also  $Re$  dependent (or a combination of both). A similar plot for  $K$  is made using the data generated by using local  $Nu$  and  $Sh$  that scale as  $Re^{0.62}$  in Figure 4. As seen in this Figure, the velocity scalings here are very close to those obtained from experimental data. The exponents of space velocity in  $K$  correlations for CO and HC are found to be 0.6548 and 0.6098 respectively which compare very well with corresponding values of 0.6355 and 0.6182 obtained experimentally [18].

From Figures 3 and 4, it is evident that the  $Re$  dependence of the effective Sherwood number is not a consequence of the variations in flow non-uniformity in the channels with increasing flow rate. The data in Figure 4 is replotted in terms of the effective  $Sh$  (for the monolith) and the average  $Re$  in Figure 5. As seen, the computed effective Sherwood numbers are slightly lower than those

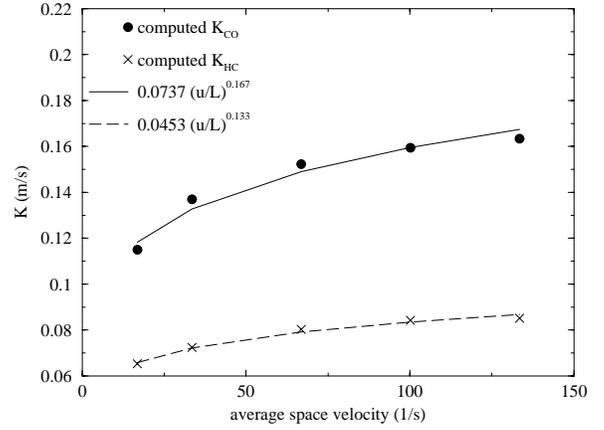


Figure 3: Effective mass transfer correlation predicted using laminar correlations for local  $Sh$  and  $Nu$

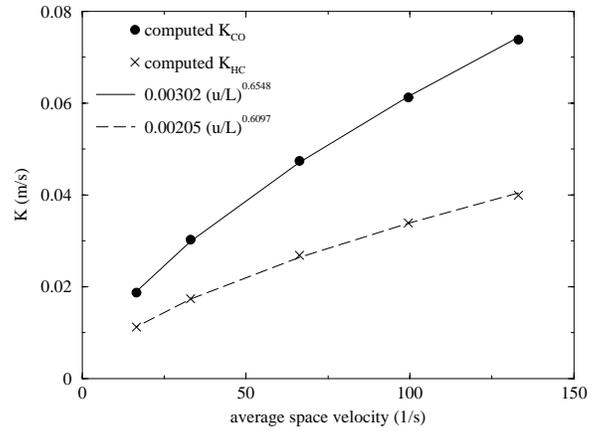


Figure 4: Effective mass transfer correlation predicted using  $Sh$  and  $Nu$  correlation derived from experiments

obtained experimentally but they scale similarly with the average  $Re$ . Also, the local and effective  $Sh$  are found to have near similar functional relationships with channel Reynolds number and average channel Reynolds number respectively. The discretization errors in the numerical scheme or the use of isothermal flow assumption while obtaining the experimental  $Sh$  could have contributed to the differences between the experimental and computed values. But it is also likely that numerical constants in scaling laws for local and effective  $Sh$  (in terms of local and average  $Re$  respectively) are slightly different.

The new scaling for  $Sh$  affects the functional relationship between conversion efficiency and the space velocity drastically. If laminar correlations for  $Sh$  are used (in which case local  $Sh$  is nearly constant at most locations), equation(6) results in the following relationship.

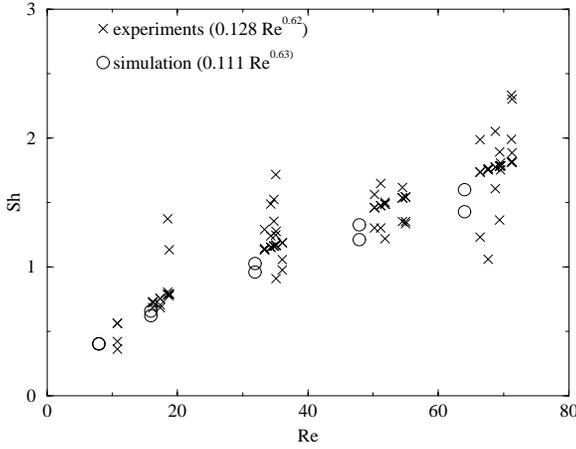


Figure 5: Comparison of predicted and experimental variations in effective  $Nu$  with average  $Re$

$$\theta \sim 1 - \exp(\alpha u^{-1}) \quad (8)$$

$\alpha$  here is a parameter independent of the velocity. On the other hand, if the  $Sh \sim Re^{0.62}$  scaling is used, the dependence of  $\theta$  on  $u$  becomes weaker.

$$\theta \sim 1 - \exp(\beta u^{-0.38}) \quad (9)$$

In the equation above,  $\beta$  is a velocity independent parameter. Thus the level of non-uniformity in the channel conversion efficiency across the face of the monolith is reduced. Figure 6 shows the (normalized) deviations of local efficiencies from the mean along the radial direction.

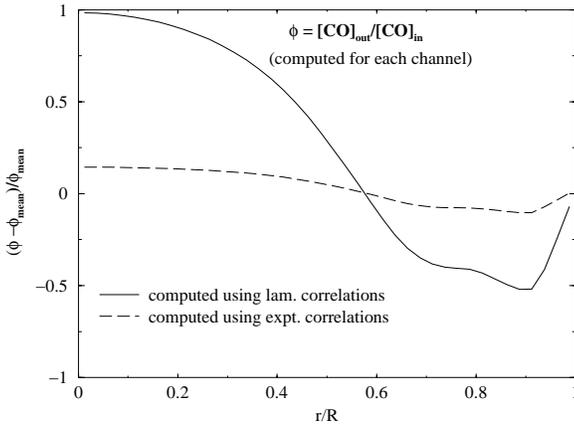


Figure 6: Non-uniformities of conversion efficiencies across the face of the monolith

As expected, the individual channel efficiencies are much closer to the mean when the experimental scaling is used for modeling mass transfer. So, the level of flow non-uniformity is now of lesser consequence. This would mean that the conversion efficiencies predicted using a one-dimensional, equivalent single channel, reactor models would perhaps be closer to those predicted using a multi-channel model. This hypothesis is tested by comparing the overall efficiencies predicted by the multi-channel model and a single channel model for the case with most non-uniform flow in the monolith. The time-evolutions of efficiencies from the two models are shown in Figure 7. The difference in the predictions is found to be as high as 10% during the transient phase. The differences are more pronounced for predictions of HC conversion than for CO conversion. The precise reasons for this are yet unclear. Both for CO and HC, the one-dimensional model predicts steady state conversion efficiencies that are within 1% of the corresponding predictions using the multi-channel model.

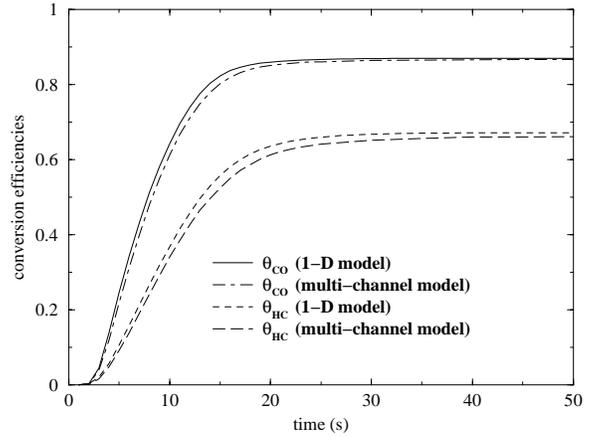


Figure 7: Comparison of conversion efficiencies predicted by the present multi-channel model and a equivalent single channel model

The flow distributions at various times before light-off in simulation with the highest flow rate (and experimental correlations for heat and mass transfer) are shown in Figure 8. The reasons for minor but noticeable changes in the flow distribution with time while the monolith is being heated by the exhaust have already been discussed by Chakravarthy *et al.* [33].

The overall level of non-uniformity is nearly the same at all times. However, unlike at steady state conditions when the substrate temperature is nearly uniform everywhere, the solid temperature (i.e., temperature of the channel walls) is quite non-uniform during the transient phase. This leads to radially non-uniform conversion in the mono-

lith. The assumption in the single channel model is that the solid temperature is uniform along the radial direction and lightoff occurs at the same time in all channels. The conversion efficiencies increase rapidly across the lightoff transition to reach an asymptotic values determined by the mass transfer rates. The lightoff transitions in all the channels of the multi-channel simulation do not occur at the same time. Hence, the overall efficiencies increase more gradually than in the single channel model where all lightoff events (and jumps in efficiency) are assumed to coincide.

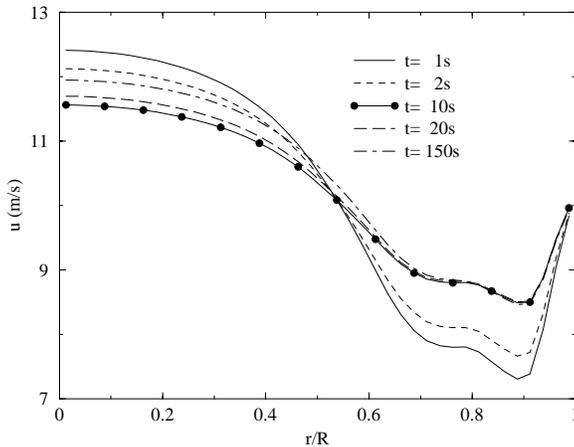


Figure 8: Evolution of flow distribution during the pre-light-off transient phase of operation

## CONCLUSIONS

Our simulation results for diesel exhaust indicate that observed mass transfer variations with flow for diffusion-limited oxidation of CO and HC are probably the result of intra-channel effects as opposed to flow distribution changes upstream from the monolith. Specifically, it appears that the actual intra-channel mass and heat transport in monoliths may retain some of the characteristic Reynolds number dependence seen in packed bed reactors. We conjecture that this behavior may be due to surface unevenness or porosity in the washcoat. Until the detailed mechanisms responsible for this deviation from laminar channel flow are better understood, oxidation reactor simulations should be based on experimental correlations for mass and heat transfer. It appears that for simulating steady-state conversion of HC and CO, a single-channel model provides adequate detail (as compared to a multi-channel model). For light-off simulations however, a multi-channel model is more appropriate due to the large thermal gradients that can occur.

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## NOMENCLATURE

$C_g$	gas phase chemical concentrations ( $mol/m^3$ )
$C_s$	solid phase chemical concentrations ( $mol/m^3$ )
$Da$	Damkohler number
$D_h$	hydraulic diameter ( $m$ )
$K$	mass transfer coefficient ( $m/s$ )

$L$	length of the monolith ( $m$ )
$Nu$	Nusselt number
$R$	radius of the monolith ( $m$ )
$r$	radial distance from the center-line ( $m$ )
$Re$	Channel Reynolds number
$R_{CO}$	reaction rate for CO oxidation ( $mol/m^3s$ )
$R_{HC}$	reaction rate for hydrocarbon oxidation ( $mol/m^3s$ )
$S$	hydraulic surface area per unit volume ( $m^2/m^3$ )
$Sh$	Sherwood number
$T$	temperature ( $K$ )
$u$	axial velocity in the channels ( $m/s$ )
$u_o$	average $u$ at the inlet face of the monolith ( $m/s$ )
$x$	axial distance from the inlet face of the monolith ( $m$ )
$\epsilon$	hole fraction
$\phi$	$1 - \theta$
$\theta$	conversion efficiency