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Hybrid flow modelling approach applied to automotive catalysts

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ABSTRACT

Catalytic converters are employed in automotive emissions after treatment for the reduction of pollutants. Flow behaviour in a catalyst system may be modelled using computational fluid dynamics. This study concerns a planar catalytic converter system with a wide-angled planar diffuser under steady flow conditions, in which the flow is approximately two-dimensional. The catalyst monolith is modelled using a novel hybrid approach. Individual channels at the entrance to the substrate provide an accurate description of flow upon entrance to the monolith. A porous region then applies the macroscopic pressure drop on the fully developed flow. Flow predictions are compared with experimental data in the diffuser and downstream of the monolith. Overall, the hybrid model improves upon the separate use of the two approaches. The variance of downstream velocity predictions from experimental data is decreased by up to 50% compared to the porous medium model, whilst the computational demand is reduced by approximately one order of magnitude compared to the individual channels model.

1. Introduction

Catalytic converters are employed in the automotive industry for compliance with emissions regulations. The catalyst is commonly a monolith comprised of many parallel channels of small hydraulic diameter (∼1 mm). A washcoat applied to the channel walls is deposited with precious metals, creating a large surface area for the reaction of exhaust gases. A wide-angled diffuser connects the exhaust pipe to the front face of the catalyst, resulting in flow separation in the diffuser and non-uniformly distributed flow in the catalyst, as shown in Fig. 1.

Non-uniform flow entering the catalyst affects its conversion efficiency [1–3], degradation rate [2] and light-off performance [4]. The level of flow maldistribution is a key factor in the design process of catalytic converters and is commonly used in the automotive industry. A relatively simple measure of conversion efficiency can then be obtained for post light-off conditions where reactions are mass-transfer limited [3,5,6]. Conversion efficiency η as a function of flow velocity can then be described by Eq. (1) [5]:

$$\eta = 1 - \exp\left(\frac{-4Lk_c}{u_c d_h}\right), \tag{1}$$

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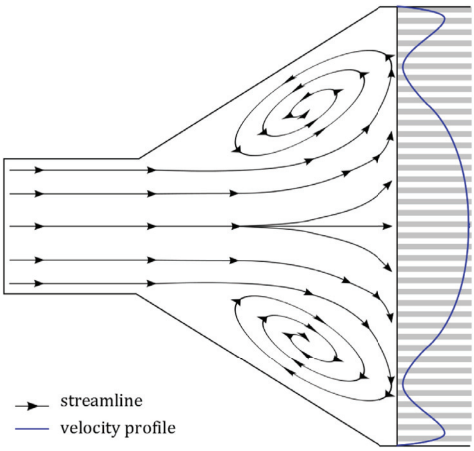
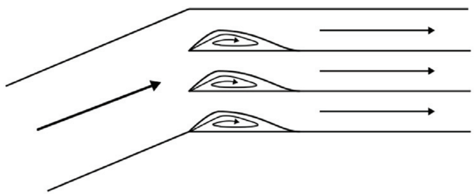
Nomenclature

ΔP	axial pressure drop
ΔP^*	non-dimensional axial pressure drop, $\Delta P/\frac{1}{2}\rho u_c^2$
ΔP_{obl}	axial pressure drop due to oblique flow
η	channel conversion efficiency
μ	dynamic viscosity
ν	kinematic viscosity, μ/ρ
ψ	non-uniformity index
ρ	density
d_h	hydraulic diameter of channel
f	Fanning friction factor
$GHSV$	gas hourly space velocity
k_c	mass transfer coefficient
L	length of monolith
$\dot{m}$	mass flow rate
N	number of mesh elements
$\mathbf{P}_{\mathrm{i}}$	porous inertial resistance tensor
$\mathbf{P}_{\mathrm{v}}$	porous viscous resistance tensor
Re	inlet Reynolds number, $\rho U_{\mathrm{in}} d/\mu$
Re_c	channel Reynolds number, $\rho u_c d_h/\mu$
U	mean axial velocity downstream of monolith
u	axial velocity
u^*	reference velocity, computed from wall law
u_c	channel velocity
U_{in}	inlet velocity
V	variance of prediction from experimental data
v	transverse velocity
X^+	non-dimensional distance along channel, $L/d_h\mathrm{Re}_c$
y	distance from wall
y^+	non-dimensional distance from wall, yu^*/ν
d	nozzle hydraulic diameter

where L is the length of the monolith channel, u_c is the channel velocity, d_h is the channel hydraulic diameter, and k_c is the mass transfer coefficient which may be determined theoretically [7]. Such an expression may then be readily integrated across the predicted velocity profile to obtain an estimation of overall conversion efficiency. An example of this is found in



(a) Flow field in diffuser and typical velocity profile inside monolith



(b) Recirculation bubbles formed at channel walls

Fig. 1. Example of flow behaviour in a catalytic converter system.