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Validity and scalability of an asymptotically reduced single-channel model for full-size catalytic monolith converters

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ABSTRACT

A catalytic monolith converter usually comprise several hundred or thousands of channels. Mathematical modeling that seek to resolve the coupled transport phenomena – mass, momentum, species and heat – on a discrete-channel scale is a computationally-challenging task. In this context, we present an efficient approach to overcome the difficulties in the modeling of a monolith converter. In short, we establish the condition for validity of a fast and efficient reduced single monolith channel model for modeling multiple channels. The reduced model is then verified for an assembly of two channels with the full set of equations; good agreement is found for typical monolith material and operating conditions indicating the ability of the reduced model to capture conjugate heat transfer across channels. We then study the computational efficiency of the reduced model for monoliths comprising $O(10^4)$ channels. The computational penalty for reduced model is much less as compared to the full model, making it a possible candidate for detailed monolith simulations.

1. Introduction

Catalytic monolith converters have been used for nearly four decades to reduce the toxicity of exhaust gases from the internal combustion engine powering automotive/machines [1–3]. Typically, a monolithic converter comprises several hundreds or thousands of slender, parallel, and straight channels as shown in Fig. 1. The engine exhaust flow through the small channels and undergo catalytic conversion.

Mathematical modeling and simulation have found widespread use in the research and development of monolith converters [1,4,6–9]. The mathematical modeling that seeks to provide geometrical resolution and resolve the essential physics that occur within a monolith has been found to be a challenging task due to the following reasons:

- Three-dimensional nature of the constituent channels: Monolith channels are manufactured in various cross-sectional shapes, including circles, squares, hexagon, triangles and sinusoids. Three-dimensional (3D) models are necessary for all these geometries – except for the circle-shaped cross-section.
- Multiple coupled transport phenomena: Equations governing conservation of mass, momentum, species, and energy inside each channel and between channels result in coupled non-linear partial differential equations (PDEs).

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List of symbols

A	pre-exponential Arrhenius factor, mol K m^{-3} s^{-1}
a	cross-sectional area, m^2
c_p	specific heat capacity, J kg^{-1} K^{-1}
$\mathfrak{D}_i^0$	constants for effective diffusivity relations, kg m s^{-3} $K^{-1/2}$
D_{ij}^{eff}	effective diffusivity of species i, m^2 s^{-1}
E_a	activation energy, J mol^{-1}
$\hat{\mathbf{e}}_x, \hat{\mathbf{e}}_y, \hat{\mathbf{e}}_z$	coordinate vectors
$\mathbf{e}$	heat flux, W m^{-1}
G	inhibition term, K
H	thickness, m
$\triangle H$	enthalpy of the reaction, J mol^{-1}
$\triangle H_a$	adsorption enthalpy, J mol^{-1}
$\mathbf{I}$	unit tensor
$\mathfrak{K}_i^{o,r}, \mathfrak{k}_i^{o,r}$	constants for inhibition term expression
k	thermal conductivity, W m^{-1} K^{-1}
L	length of the channel, m
M	molecular mass, kg mol^{-1}
$\mathbf{n}_i$	mass flux of species i, mol m^{-2} s^{-1}
$\hat{\mathbf{n}}$	unit normal to a given plane
p, $\tilde{p}$	pressure and its dimensionless form, Pa, -
Q	mass flow rate, kg s^{-1}
R	gas constant, J mol^{-1} K^{-1}
r	rate of reaction, mol m^{-3} s^{-1}
S	source term
$T, \tilde{T}$	temperature and its dimensionless form, K, -
$\hat{\mathbf{t}}$	unit tangent to a given plane
$\mathbf{v}, u, v, w$	velocities, m s^{-1}
$\mathfrak{v}$	diffusion volume, m^3 mol^{-1}
y_i	molar fraction of species i
x, y, z	coordinates, m

Greek

α	stoichiometric coefficient
ε	porosity
κ	permeability, m^2
μ	dynamic viscosity, kg m^{-1} s^{-1}
ρ	density, kg m^{-3}
ς	vorticity, s^{-1}
$\boldsymbol{\tau}$	viscous momentum-flux tensor, N m^{-2}
$\boldsymbol{\phi}$	combined momentum-flux tensor, N m^{-2}
ω_i	mass fraction of species i

Superscripts

eff	effective
in	inlet
o	oxidation reaction
r	reduction reaction
ref	reference

Subscripts

CO	carbon monoxide
CO_2	carbon dioxide
C_3H_7	hydrocarbon representative
eff	effective
fc	flow channel
g	gas phase
H_2	hydrogen