# Towards computationally-efficient modeling of transport phenomena in three-dimensional monolithic channels

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**ABSTRACT**

In general, three-dimensional (3D) non-isothermal models for monolithic channels that seek to capture the local transport phenomena are computationally expensive. In this regard, we present a reduced model for a monolithic channel that reduces the computational cost, whilst preserving the 3D geometry and all of the essential physics – this is accomplished by exploiting the inherent slenderness of the monolith channel, coupled with scaling arguments, leading-order asymptotics and a fast space-marcher. The model takes into account conservation of mass, momentum, species and energy coupled with chemical kinetics, and is demonstrated for a three-way reaction mechanism for treatment of automotive exhaust. The results of the reduced model are verified against those of the full model and validated with axial temperature distributions for an experimental square channel. Overall, memory requirements and computing time are reduced by around 2–3 orders of magnitude as compared to the full set of equations. Finally, we discuss the suitability of the reduced model for reactor-scale modeling and extensions for transient simulations and other slender chemical engineering systems.

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## 1. Introduction

Monolithic reactors are widely used for reducing emissions through conversion of toxic by-products of combustion into less harmful substances in gasoline-powered vehicles. In addition to their well-established role as automotive converters, they represent potential alternatives in many other applications: e.g., catalytic combustion of methane, catalytic oxidation, hydrogenation or dehydrogenation of aromatic compounds, hydrogen generation for fuel cells, steam reforming of light hydrocarbons and methanol, water gas shift reactions, etc. [1,2]. Typically, a monolithic reactor – ceramic or metallic – comprises several hundreds of slender, parallel, and straight channels as shown in Fig. 1. The channels are in turn coated with a porous material that serves as a support for the catalytic materials: usually a noble metal such as platinum (Pt), rhodium (Rh) or palladium (Pd). The resulting structure provides a high surface area and gives rise to a low pressure drop in comparison with, for example, packed bed reactors.

Mathematical modeling and simulation have found widespread use in research and development of monolithic reactors: numerous mathematical models have been reported with varying degrees of complexity in terms of model dimensionality, washcoat modeling, chemical kinetics and number of species, physics and dynamics [1,3–8]. These models, as a complement

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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$^{-1/2}$ |
| $D_{ij}^{\text{eff}}$ | 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 |
| $\mathfrak{R}_i^{\text{o,r}},\ \mathfrak{f}_i^{\text{o,r}}$ | 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 |
| $T,\ \widetilde{T}$ | temperature and its dimensionless form, K, – |
| $\hat{\mathbf{t}}$ | unit tangent to a given plane |
| $\mathbf{v},\ u,\ v,\ w$ | velocities, m s$^{-1}$ |
| $\upsilon$ | diffusion volume, m$^3$ mol$^{-1}$ |
| $y_i$ | molar fraction of species i |
| $x,\ y,\ z$ | coordinates, m |

**Greek**

| | |
|---|---|
| $\alpha$ | stoichiometric coefficient |
| $\varepsilon$ | porosity |
| $\kappa$ | permeability, m$^2$ |
| $\mu$ | dynamic viscosity, kg m$^{-1}$ s$^{-1}$ |
| $\rho$ | density, kg m$^{-3}$ |
| $\varsigma$ | vorticity, s$^{-1}$ |
| $\tau$ | viscous momentum-flux tensor, N m$^{-2}$ |
| $\phi$ | combined momentum-flux tensor, N m$^{-2}$ |
| $\omega_i$ | 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 |
| $H_2O$ | water |
| i | species i |