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Reduced order multimode transient models for catalytic monoliths with micro-kinetics



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HIGHLIGHTS

- A new reduced order model is developed for monoliths with micro-kinetics.
- The multimode model is independent of the solid–fluid interfacial flux.
- The model is more accurate than twophase models for transient reacting flows.
- Traditional flux expression has limited validity for fast transients with reaction.
- Comparisons with two-phase and 1+1 dimensional models is presented.

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G R A P H I C A L A B S T R A C T

Response curve of adsorbing solute in monolith for a unit impulse input: effective velocity decreases and overall spreading increases with increase in adsorption–desorption equilibrium constant K_{eq} . The effective dispersion coefficient of adsorbing solute varies non-monotonically with K_{eq} .



ABSTRACT

We present a reduced order model for describing the transient diffusion and convection in monolith channels with diffusion, adsorption, desorption and reaction in the porous washcoat layer. Unlike the traditional two-phase or the 1(axial)+1(washcoat) dimensional models whose validity may be limited for transient reacting flows, the present multi-mode model is accurate to first order in the transverse diffusion time (t_D) and hence is valid over a much wider range of operating conditions and kinetics. We provide a physical interpretation of the various effective coefficients appearing in the reduced order model. For the case of inert and non-reacting solutes, we obtain effective transport coefficients and relate them to experimental observations. For the steady-state reacting case, we present a multi-mode form of the model with intra- and interphase mass transfer coefficients. In the general transient case, we show that the traditional external mass transfer coefficient concept is not applicable as the solid-fluid interfacial flux cannot be expressed in terms of concentration differences even to leading order in t_D . We also show that for transient reacting flows, the widely used two-phase and 1+1 dimensional models may lead to errors of order unity in the solid–fluid interfacial flux and order t_D in the exit concentration or moments. Finally, we apply the reduced order model to the chromatographic method to relate the first and second moments to the effective diffusivities and kinetic parameters and compare the results with those obtained from the traditional two-phase models.

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Nomenclature

		P	
Roman l	etters	r	radial coordinate
а	radius of the tube	R_a	adsorption rate per unit pore surface are
anc	area (available for adsorption) unit volume of washcoat	R _d	desorption rate per unit pore surface are
Ao	cross-sectional area of flow channel	R_w	reaction rate per unit pore surface area
A _o	cross-sectional area of washcoat	$\widetilde{R_{W}}$	homogeneous global reaction (based or
Γ_{Ω_w}	concentration of adsorbed species (based on unit pere		ume) in washcoat
Ca	concentration of adsorbed species (based on unit pore	P	bydraulic radius for flow channel
	surface area)	R_{Ω_f}	offective (diffusion) length scale in wash
c _{a0}	initial concentration of adsorbed species (based on unit	K_{Ω_w}	effective (ultrusion) length scale in wash
	pore surface area)	Sne	external Snerwood number
CaT	total concentration of sites (based on unit pore surface	Sho	overall Sherwood number
	area)	$Sh_{\Omega i}$	internal Sherwood number
Cf	solute concentration in fluid phase	t	real time
Cmf	cupmixing concentration	t _{ads}	adsorption time constant
Cmf in	inlet solute concentration in fluid phase	t _C	convection diffusion time
Ca-	initial solute concentration in fluid phase	tn	transverse diffusion time in flow channe
C _{f0}	some reference concentration in fluid phase	tan	desorption time constant
Cref	some reference concentration in nuit phase	t	transverse diffusion time in washcoat
C_{S}	solute concentration at fluid-washcoat interface	t Dw	reaction time constant
Cw	concentration in washcoat	L _R	fluid value ity in the avial direction (direction)
C_{w0}	initial solute concentration in washcoat	u_f	fluid velocity in the axial direction (dime
$\langle c_a \rangle_w$	cross-sectionally averaged concentration (based on unit	$\langle u \rangle_f$	cross-sectional averaged velocity in flui
	pore surface area) of adsorbed species in washcoat		axial direction (dimensional)
$\widetilde{C_a}$	concentration of adsorbed species per unit volume in	$\langle u \rangle_{eff}$	effective velocity appearing in reduced
u	washcoat	55	monolith scale
$\langle \widetilde{\mathbf{c}} \rangle$	cross-sectionally averaged concentration of adsorbed	$\langle u \rangle_0$	effective velocity appearing in reduced
$\langle \mathbf{c}_a \rangle_w$	species unit volume in washcoat	(17)0	monolith scale to the leading order in $t_{\rm D}$
(-)	species unit volume in washcoat	v	coordinate along the length of the reactor
$\langle c \rangle_f$	cross-sectionally averaged concentration in huid phase	A	coordinate along the length of the reactor
$\langle c \rangle_{W}$	cross-sectionally averaged concentration in washcoat		
$\langle c_s \rangle$	peripheral averaged concentration at fluid-washcoat	Greek l	etters
	interface	\mathcal{E}_{WC}	porosity of the washcoat
D _f	molecular diffusivity of solute in fluid phase	ϕ_d	Thiele modulus based on desorption rate
d_h	hydraulic diameter of flow channel	ϕ_w	Thiele modulus based on reaction rate
D _{off}	effective Taylor diffusivity in the monolith	$\phi_{\rm off}$	Thiele modulus based on effective reacti
D _T	Taylor diffusivity in the flow channel	v	volume capacity of the washcoat
D	molecular diffusivity of solute in washcoat	ŕ	ratio of pet (adsorption \pm volumetric) of
D _W E	PTD (residence time distribution) curve	1	washcoat to that of fluid phase
E c	All (residence time distribution) curve		washcoat to that of hulu phase
sat =	adsorption-desorption isotnerm	Yeq	adsorption capacity of the washcoat
=	interfacial molecular flux at fluid-washcoat interface	γ_w	volume ratio of washcoat to the flow cha
$\langle J \rangle =$	peripheral averaged interfacial molecular flux at fluid–	θ	azimuthal coordinate
	washcoat interface	θ_s	fraction of adsorbed sites occupied
$\langle I \rangle_{ss} =$	Peripheral averaged interfacial molecular flux at fluid-	\varkappa_e	exit conversion
0733	washcoat interface at steady-state	$\lambda =$	ratio of washcoat thickness to radius of
k.	adsorption rate constant	Δ	Λ_{-} transverse coefficient appearing in
μ.	desorption rate constant	1 mj , 1	model
к _d	desorption rate constant in monolith		dimensionless offective dispersion coeffe
K _{eff}	effective reaction rate constant in monontin	Λ_{eff}	dimensionless effective dispersion coeffi-
<i>k</i> _{ext}	external mass transfer coefficient	μ	ratio of solute diffusivities in fluid to wa
k_w	reaction rate constant	μ_2	second central moment (temporal) of exi
k _{w.eff}	global reaction rate constant in washcoat	τ	dimensionless time (non-dimensionaliz
$k_{ff}, \tilde{k}_{fw}, k$	$k_{wf}, k_{ww}, k_{sf}, k_{sw}, k_{sf1}, k_{sw1}, k_{f0}$ coefficients in reduced order		tion time t_c)
<u>)</u> , , , , , , , , , , , , , , , , , , ,	model	Ω	overall cross-section (flow channel + was
k	internal mass transfer coefficient	Oc	cross-section of flow channel
k.	overall mass transfer coefficient	0	cross-section of washcoat
κ ₀ Ι	Longth of the monolith	52 _W	CI035-SECTION OF WASHCUAL
L	Length of the monolul		
m_k	<i>k</i> -tn moment (temporal) of exit concentration	Operate	ors
\mathbf{n}_{Ω_f}	unit normal vector to $\partial\Omega_f$	∇^2	transverse Laplacian operator (dimension
\mathbf{n}_{Ω_w}	unit normal vector to $\partial \Omega_w$	$\langle \rangle_{f}^{\perp}$	inner product (averaged) over flow chan
Pof	perimeter of the fluid-washcoat interface		inner product (averaged) over washcoat
	-	\/ <i>W</i>	miller produce (averagea) over washeodt

р	transverse Peclet number		
r	radial coordinate		
Ra	adsorption rate per unit pore surface area		
R _d	desorption rate per unit pore surface area		
R_w	reaction rate per unit pore surface area		
R_w	homogeneous global reaction (based on per unit vol-		
	ume) in washcoat		
R_{Ω_f}	hydraulic radius for flow channel		
R_{Ω_w}	effective (diffusion) length scale in washcoat		
Sh _e	external Sherwood number		
Sho	overall Sherwood number		
$Sh_{\Omega i}$	internal Sherwood number		
t	real time		
t _{ads}	adsorption time constant		
t _C	convection diffusion time		
t _D	transverse diffusion time in flow channel		
t _{des}	desorption time constant		
t _{Dw}	transverse diffusion time in washcoat		
t_R	reaction time constant		
u_f	fluid velocity in the axial direction (dimensional)		
$\langle u \rangle_f$	cross-sectional averaged velocity in fluid phase in the		
()	axial direction (dimensional)		
$\langle u \rangle_{eff}$	effective velocity appearing in reduced order model at		
()	inononin scale		
$\langle u \rangle_0$	enective velocity appearing in reduced order model at monolith scale to the leading order in t		
v	r_{D}		
Λ	coordinate along the length of the reactor (unitensional)		
Crook lat	and the second se		
Greek lett	ers		
Greek lett	ers porosity of the washcoat Thiele modulus based on desorption rate		
Greek lett ε_{wc} ϕ_d	ers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_w	ers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_{eff}	ers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_{eff} γ Γ	ers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the		
$\begin{array}{l} Greek \ lett \\ \varepsilon_{wc} \\ \phi_d \\ \phi_w \\ \phi_{eff} \\ \gamma \\ \Gamma \end{array}$	eers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_{eff} γ Γ γ_{eff}	ters porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_{eff} γ Γ γ_{eq} $\gamma_{}$	porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_{eff} γ Γ γ_{eq} γ_w θ	porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_{eff} γ Γ γ_{eq} γ_w θ θ_s	porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_{eff} γ Γ γ_{eq} γ_w θ θ_s \varkappa_e	porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion		
Greek lett ε_{wc} ϕ_d ϕ_w ϕ_{eff} γ Γ γ_{eq} γ_w θ θ_s \varkappa_e $\lambda =$	porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion ratio of washcoat thickness to radius of flow channel		
Greek lett ε_{wc} ϕ_d ϕ_{w} ϕ_{eff} γ Γ γ_{eq} γ_w θ θ_s χ_e $\lambda =$ $\Lambda_{mf}, \Lambda_{mv}$	porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion ratio of washcoat thickness to radius of flow channel v_{1} , Λ_{q} transverse coefficient appearing in reduced order		
Greek lett ε_{wc} ϕ_d ϕ_{w} ϕ_{eff} γ Γ γ_{eq} γ_w θ_s λ_{e} λ_{mf} , Λ_{mv}	porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion ratio of washcoat thickness to radius of flow channel w, Λ_a transverse coefficient appearing in reduced order model		
Greek lett ε_{wc} ϕ_d ϕ_{w} ϕ_{eff} γ Γ γ_{eq} γ_w θ θ_s χ_e $\lambda =$ $\Lambda_{mf}, \Lambda_{mv}$ Λ_{eff}	pers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion ratio of washcoat thickness to radius of flow channel w_i , Λ_a transverse coefficient appearing in reduced order model dimensionless effective dispersion coefficient		
Greek lett ε_{wc} ϕ_d ϕ_{w} ϕ_{eff} γ Γ γ_{eq} γ_w θ θ_s χ_e $\lambda =$ $\Lambda_{mf}, \Lambda_{mv}$ Λ_{eff} μ	pers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion ratio of washcoat thickness to radius of flow channel w, Λ_a transverse coefficient appearing in reduced order model dimensionless effective dispersion coefficient ratio of solute diffusivities in fluid to washcoat		
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$ \begin{array}{l} Greek \ lett \\ \varepsilon_{wc} \\ \phi_d \\ \phi_{w} \\ \phi_{eff} \\ \gamma \\ \Gamma \\ \gamma \\ \Gamma \\ \gamma \\ \theta_s \\ \chi_e \\ \lambda = \\ \Lambda_{mf}, \ \Lambda_{mv} \\ \Lambda_{eff} \\ \mu \\ \mu_2 \\ \tau \\ \Omega \\ \Omega_w \end{array} $	pers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion ratio of washcoat thickness to radius of flow channel w, Λ_a transverse coefficient appearing in reduced order model dimensionless effective dispersion coefficient ratio of solute diffusivities in fluid to washcoat second central moment (temporal) of exit concentration dimensionless time (non-dimensionalized by convec- tion time t_c) overall cross-section (flow channel + washcoat) cross-section of washcoat		
Greek lett ε_{wc} ϕ_d ϕ_{w} ϕ_{eff} γ Γ γ_{eq} γ_w θ_s χ_e $\lambda =$ $\Lambda_{mf}, \Lambda_{mv}$ Λ_{eff} μ μ_2 τ Ω Ω_w	pers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion ratio of washcoat thickness to radius of flow channel w, Λ_a transverse coefficient appearing in reduced order model dimensionless effective dispersion coefficient ratio of solute diffusivities in fluid to washcoat second central moment (temporal) of exit concentration dimensionless time (non-dimensionalized by convec- tion time t_c) overall cross-section (flow channel + washcoat) cross-section of washcoat		
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$ \begin{array}{l} Greek \ lett \\ \varepsilon_{wc} \\ \phi_d \\ \phi_{w} \\ \phi_{eff} \\ \gamma \\ \Gamma \\ \end{array} \\ \Gamma \\ \gamma_{eq} \\ \gamma_w \\ \theta_s \\ \chi_e \\ \lambda = \\ \Lambda_{mf}, \ \Lambda_{mv} \\ \Lambda_{eff} \\ \mu \\ \mu_2 \\ \tau \\ \Omega \\ \Omega_f \\ \Omega_w \end{array} $	pers porosity of the washcoat Thiele modulus based on desorption rate Thiele modulus based on reaction rate Thiele modulus based on effective reaction rate volume capacity of the washcoat ratio of net (adsorption + volumetric) capacity of the washcoat to that of fluid phase adsorption capacity of the washcoat volume ratio of washcoat to the flow channel azimuthal coordinate fraction of adsorbed sites occupied exit conversion ratio of washcoat thickness to radius of flow channel w, Λ_a transverse coefficient appearing in reduced order model dimensionless effective dispersion coefficient ratio of solute diffusivities in fluid to washcoat second central moment (temporal) of exit concentration dimensionless time (non-dimensionalized by convec- tion time t_c) overall cross-section (flow channel + washcoat) cross-section of washcoat		

1. Introduction

Mathematical models describing the steady-state and transient behavior of chemical reactors and separation columns are obtained by combining the various conservation laws with the constitutive equations for the rate processes. When smaller scale processes such as diffusion, adsorption, desorption and reaction are included, and inlet conditions vary with time, these models are usually

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