



# Heat and mass transfer coefficients and bifurcation analysis of coupled homogeneous-catalytic reactions

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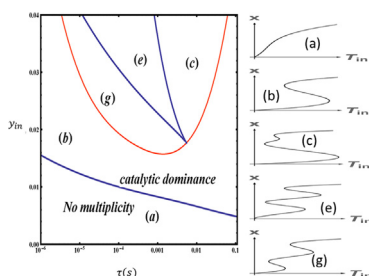
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## HIGHLIGHTS

- A 3-mode model for coupled homogeneous-catalytic reactions is developed.
- Various inter and intra-phase heat/mass transfer coefficients are determined.
- Bifurcations occurring during catalytic oxidation of propane are analyzed.
- Maximum temperature rise in catalytically assisted combustion is determined.

## GRAPHICAL ABSTRACT

Phase diagram for classification of various bifurcations that could occur in the catalytically assisted combustion of propane in a monolith. The letter in each region of the space time-inlet mole fraction plane denotes the type of bifurcation diagram (of conversion versus inlet temperature) in that region.



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## ABSTRACT

We analyze the problem of flow in a channel with homogeneous reaction(s) in the bulk and catalytic reaction(s) on the wall and develop a reduced order 3-mode model in terms of mixing-cup, wall and channel cross-section averaged concentrations and temperatures. Unlike classical two-phase models that contain a single inter-phase transfer coefficient, the 3-mode models contain three transfer coefficients representing the inter and intra-phase heat/mass transfer. We determine the dimensionless inter and intra-phase transfer coefficients (Nusselt and Sherwood numbers) that appear in the reduced order model as a function of position (Graetz coordinate), Peclet and local Damköhler numbers. We illustrate the use of the reduced order models to determine the bifurcation (ignition/extinction) features of coupled homogeneous-catalytic reactions in monolith channels and gauze reactors using propane combustion as an example. The 3-mode model is also used to analyze and determine the maximum temperature in catalytically assisted combustion in a channel in the convection dominated limit.

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## 1. Introduction and literature review

Catalytic combustion and catalytic partial oxidation systems have been analyzed by many investigators using theoretical, computational and experimental techniques over the past four

decades. The strong chemical as well as thermal coupling between the homogeneous and catalytic chemistries, very short space times (of the order of milliseconds) and high adiabatic temperature rise (500 to over 1500 °C) may lead to complexity of the solutions space (with various ignitions, extinctions, extremely thin boundary layers, spatial and temporal patterns), and make the analysis of these systems rather difficult. The current practice in modeling of these systems is dominated by micro-kinetic models for homoge-

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## Nomenclature

### Roman letters

$C$	fluid concentration
$c$	dimensionless fluid concentration
$\langle c \rangle$	cross-section averaged concentration
$c_m$	mixing-cup concentration
$c_s$	wall concentration
$C_{pf}$	fluid phase heat capacity
$D_m$	diffusion coefficient in the fluid phase
$Da$	Damköhler number for the homogeneous reaction
$Da_c$	Damköhler number for the catalytic reaction
$E_a$	activation energy for the homogeneous reaction
$E'_a$	activation energy for the catalytic reaction
$k_f$	fluid thermal conductivity
$k_{ex}$	effective thermal conductivity in the direction of flow
$k_h$	first order rate constant for the homogeneous reaction
$k_c$	first order rate constant for the catalytic reaction
$L$	length of the channel
$a$	length along the first transverse coordinate
$b$	length along the second transverse coordinate
$Le_f$	fluid Lewis number
$Nu_\Omega$	interphase Nusselt number
$\tilde{N}u_\Omega$	intrapphase Nusselt number due to cross-coupling
$Nu_{i\Omega}$	intrapphase Nusselt number
$P$	transverse Peclet number
$Pe$	axial Peclet number
$Pe_r$	radial Peclet number
$Sh_\Omega$	interphase Sherwood number
$\tilde{S}h_\Omega$	intrapphase Sherwood number due to cross-coupling
$Sh_{i\Omega}$	intrapphase Sherwood number
$T$	fluid temperature
$T_{in}$	inlet fluid temperature
$\bar{u}$	average fluid velocity in the channel
$x'$	coordinate along the length of the channel (dimensional)
$y'$	first transverse coordinate (dimensional)

$z'$	second transverse coordinate (dimensional)
$x$	coordinate along the length of the channel (dimensionless)
$y$	first transverse coordinate (dimensionless)
$z$	second transverse coordinate (dimensionless)
$X$	dimensionless coordinate along the length of the channel normalized with the transverse Peclet number

### Greek letters

$\rho$	density
$\alpha$	aspect ratio
$\beta$	dimensionless adiabatic temperature rise
$\gamma_h$	dimensionless activation energy for the homogeneous reaction
$\gamma_c$	dimensionless activation energy for the catalytic reaction
$\epsilon_f$	fraction of channel cross-section open to flow
$\zeta$	dimensionless coordinate along the length of the channel normalized with the axial Peclet number
$\eta$	Graetz coordinate
$\theta$	dimensionless temperature
$\langle \theta \rangle$	cross-section averaged temperature
$\theta_m$	dimensionless mixing cup temperature
$\theta_s$	dimensionless temperature at the surface
$\lambda$	ratio of effective thermal conductivity in the direction of flow to fluid thermal conductivity
$\phi$	Thiele modulus for the homogeneous reaction
$\phi_c$	Thiele modulus for the catalytic reaction

### Subscripts and superscripts

$f$	fluid phase
$s$	solid phase
$m$	cup-mixing

neous reactions or CFD approaches to produce direct numerical studies and a substantial literature using such approaches has accumulated. Since CFD or micro-kinetic modeling are not the subject of the present paper, we provide here only a representative list of recent papers that use CFD or micro-kinetic models: Maestri et al. [1,2], Sun et al. [3], Karagiannidis et al. [4], Janardhanan and Deutschmann [5], Deutschmann et al. [6], Carroni et al. [7], and Salomons et al. [8]. There exist only a limited number of studies that analyzed the bifurcation features of such systems e.g. Song et al. [9] and Vlachos et al. [10]. Comprehensive bifurcation analyses of these systems have been rare (aside from some recent work, e.g. Alam et al. [11]). One reason for this is that models with detailed chemistry or hydrodynamics are not suitable for computational bifurcation analysis due to presence of exponentially thin boundary or internal layers requiring extremely fine mesh resolutions to avoid spurious solutions. Therefore, it is desirable to develop reduced order models (analogous to the classical two-phase models with only catalytic reactions occurring) that predict the bifurcation features while being relatively computationally inexpensive. In the past, the transfer coefficient concept has been used successfully to simplify the transverse (local) gradients using two concentration and/or temperature modes (e.g. mixing-cup in fluid phase and wall or solid–fluid interfacial) and develop such low-dimensional models of monolith reactors with only catalytic reaction (e.g. Groppi et al., [12], Hayes et al., [13], Gupta and Balakotaiah, [14], Di Benedetto et al., [15] and Gianni et al., [16]). The extension of this approach to include homogeneous reactions

is non-trivial and has not been attempted in the prior literature, and is the main focus of the present work. Specifically, we consider the problem of flow in a channel with homogeneous reaction(s) in the fluid phase and catalytic reaction(s) on the wall and show that it can be reduced to a low-dimensional form with three concentration (temperature) modes to measure the transverse (local) gradients across the channel, namely, the mixing-cup, wall (or fluid–solid interface) and cross-section averaged values. The latter third mode is not needed when only catalytic reaction is present but is essential in the presence of homogeneous chemistry, as the homogeneous reaction rates in the reduced order model are evaluated at this value. Further, while there is only a single mass (heat) transfer coefficient to describe the local gradient (and the transfer between the bulk and the solid–fluid interface) in the absence of homogeneous chemistry, the coupled problem requires three such transfer coefficients (to describe both the inter and intra-phase gradients). Thus, the major goals of this work are (i) to demonstrate the procedures and obtain reduced order models of coupled homogeneous-heterogeneous reaction systems (ii) to determine the expressions for the various heat and mass transfer coefficients that appear in the reduced order models, and (iii) to illustrate the use of the reduced order models in the bifurcation analysis of these systems.

In the next section, we formulate a mathematical model for describing the steady-state behavior of a system with flow in a channel and with coupled homogeneous-catalytic chemistry. We also consider various limiting cases of this model that are helpful

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