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Two-dimensional analytical investigation of coupled heat and mass transfer and entropy generation in a porous, catalytic microreactor

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ABSTRACT

Influences of the solid body of microreactors (or the microstructure) upon the transfer processes and hence on the performance of microreactors have been recently emphasised. Nonetheless, the subtle connections between microstructure design and micro-transport phenomena are still largely unknown. To resolve this, the current paper presents an analytical study of the advective-diffusive transport phenomena in a microreactor filled with porous media and with catalytic surfaces. The system under investigation includes the fluid and porous solid phases inside a microchannel with thick walls and subject to uneven thermal loads. The thermal diffusion of mass, viscous dissipation of the flow momentum and local thermal non-equilibrium in the porous medium are considered. The axial variations of heat and mass transfer processes are also taken into account and two-dimensional solutions of the temperature and concentration fields are provided. The local and total entropy generation within the system are further calculated. The results clearly demonstrate the major influences of thick walls on the thermal behaviour and subsequently on the mass transfer and entropy generation of the microreactor. In particular, the Nusselt number is shown to be strongly dependent upon the configuration of microstructure such that it decreases significantly by thickening the walls. The results also demonstrate that for finite Soret numbers the total irreversibility of the system is dominated by the Soret effect. The analytical results of this work can be further used for the validation of future numerical analyses of microreactors.

1. Introduction

Microreactors continue to grow in significance in various technological areas [1,2]. Broadly, these include process intensification in chemical industry [3,4], while specialised applications such as distributed fuel production [5–7] and nanoparticle generation [8] are also under development. Further, over the last two decades, there have been sustained attempts for developing micro-combustors for the purpose of micro power generation [9]. In general, microreactors have been identified as being most suitable for catalytic and highly exothermic and endothermic reactions [5,10]. This is essentially because of the fact that transport phenomena are highly enhanced in microreactors and hence thermal energy can be readily added to or removed from these systems [3,11]. Compared to macro-reactors, microreactors feature much smaller characteristic lengths and thus they are far more efficient in diffusion of heat and mass in laminar regimes [3]. Nonetheless, recent investigations indicate that optimisations of transport characteristics and second law performance of these devices are rather involved [12–14]. This is mainly due to the strong coupling of transport of heat with the microstructure of the reactor that primarily includes the surrounding walls [12,14]. In most cases, the thermal characteristics affect mass transfer and entropy generation, which are central to the optimal design and performance of the system.

Temperature fields and heat transfer in microreactors have been already examined experimentally, e.g. Refs. [15,16]. Nevertheless, the small size of microreactors makes them a challenging medium for experimental measurements and equally amenable to numerical and theoretical investigations [12,17]. Most existing modelling works in this area emphasise the influences of heat and mass transfer upon the overall operation of the reactor. In their review of thermo-hydraulics of microreactor clusters, Rebrov et al. [18] highlighted the significance of microstructure on the heat transfer behaviour of the system. They showed that heat transfer in the clusters of microreactors is heavily dependent on the materials and configurational specifications of the system [18]. Yet, the focus of their survey was on the bundles of individual microreactors and therefore they did not consider the details of heat transfer in a single reactor [18].

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Nomenclature

a_{sf}	interfacial area per unit volume of porous media
Bi	Biot number
Br'	modified Brinkman number
C	mass species concentration
C_0	inlet concentration
C_p	specific heat capacity
D	effective mass diffusion coefficient
Da	Darcy number
D_T	coefficient of thermal mass diffusion
h_1	half-thickness of the microchannel
h_2	half-height of microchannel
h_{sf}	interstitial heat transfer coefficient
H_w	wall heat transfer coefficient
k	effective thermal conductivity ratio of the nanofluid and the porous solid
k_1	thermal conductivity of wall 1
k_2	thermal conductivity of wall 2
k_{e1}	ratio of thermal conductivity of wall 1 and thermal conductivity of the porous solid
k_{e2}	ratio of thermal conductivity of wall 2 and thermal conductivity of the porous solid
k_{enf}	effective thermal conductivity of the nanofluid phase
k_{es}	effective thermal conductivity of the solid phase of the porous medium
k_R	reaction rate constant on the walls
L	length of the microchannel
M	viscosity ratio
N_{DI}	dimensionless diffusive irreversibility
N_{FF}	dimensionless fluid friction irreversibility
N_{int}	dimensionless interstitial heat transfer irreversibility
N_{nf}	dimensionless nanofluid and interstitial irreversibility
$N_{nf,ht}$	dimensionless nanofluid heat transfer irreversibility
N_s	dimensionless porous solid and interstitial irreversibility
$N_{s,ht}$	dimensionless heat transfer irreversibility
N_{w1}	dimensionless lower wall irreversibility
N_{w2}	dimensionless upper wall irreversibility
N_{pm}	dimensionless total porous medium irreversibility
N_{Tot}	dimensionless total entropy
Nu	Nusselt number
p	pressure
Pe	Peclet number
X	dimensionless axial coordinate
Pr	Prandtl number
Q	wall heat flux ratio
q''_1	lower wall heat flux
q''_2	upper wall heat flux
Re	Reynolds number
R	specific gas constant
S	shape factor of the porous medium
$\dot{S}'''_{Di}$	volumetric entropy generation due to mass diffusion
$\dot{S}'''_{FF}$	volumetric entropy generation due to fluid friction
$\dot{S}'''_{nf}$	volumetric entropy generation in the nanofluid
$\dot{S}'''_{s}$	volumetric entropy generation in the porous solid
$\dot{S}'''_{w2}$	volumetric entropy generation rate from lower wall
Sr	Soret number
T	temperature
u	nanofluid velocity
$\bar{u}$	average velocity over cross-section
Y	dimensionless transverse coordinate
x	dimensional axial coordinate
y	dimensional transverse coordinate

Greek symbols

μ	dynamic viscosity
κ	permeability
ρ	density
θ	dimensionless temperature
Φ	dimensionless concentration
ξ	aspect ratio of the microchannel
ε	porosity of the porous medium
γ	Damköhler number
ω	dimensionless heat flux defined in Eq. (40)
φ	irreversibility distribution ratio defined in Eq. (41)

Subscripts

$w1$	of the lower wall surface
$w2$	of the upper wall surface
f	base fluid
P	nanoparticles
s	of porous solid
nf	of nanofluid
1	of lower wall
2	of upper wall

In a series of numerical works, Chein and co-workers investigated the behaviour of catalytic microreactors used for fuel reforming [19–22]. Through assuming local thermal equilibrium (LTE) and Fickian mass transfer, the temperature and species fields, Nusselt number and chemical conversion rates and chemical efficiencies were computed in a micro-reformer with porous catalytic layers [19]. It was concluded that the reactor performance is dominated by the configuration of the porous catalyst [19]. This numerical work was later extended to the analyses of the effects of thermal resistance upon steam reforming of methanol in microreactors [20,21]. Chein et al. [20,21] showed that to optimise the reactor it is essential to carefully minimise the thermal resistances within the system. In a separate work, Chein et al. investigated the influences of microstructure configuration and materials on the conversion rates of a micro-reformer and made a number of design suggestions [22]. These findings clearly demonstrate the significance of accurate prediction of heat transfer rates in the design of microreactors. Importantly, almost all existing studies on transport phenomena in porous microreactors assumed LTE in the porous region [19–22]. However, recent studies on porous channels with exothermic or endothermic processes assert that an accurate prediction of the thermal behaviour of such systems warrants a local thermal non-equilibrium (LTNE) analysis [23–26]. In particular, the most recent theoretical studies of microreactors have confirmed that taking LTNE approaches are essential for the accurate prediction of the thermal and entropic behaviours of these systems [12,13].

Most microreactors consist of microchannels and therefore share their heat transfer characteristics with them. Early analyses of porous microchannels included LTE assumption e.g. [27] and LTNE investigation of microchannels have been only reported in recent years. Buonomo et al. [28] conducted an analytical LTNE study of forced convection in a porous microchannel with a rarefied gas flow. These authors [28] showed that heat transfer increases as Biot number increases and reaches asymptotic values. Through considering the viscous forces in porous microchannels,