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Numerical study of heat and mass transfer in the microwave-assisted and conventional packed bed reactors with an irreversible first-order endothermic chemical reaction

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ABSTRACT

This paper presents a numerical study on heat and mass transfer in the microwave-assisted and conventional packed bed reactors with an irreversible first-order endothermic chemical reaction. The numerical simulations have been carried out using one-dimensional heterogeneous reactor models for the both reactors. The obtained results have been compared applying the criterion of the same electrical powers utilized in the reactors. The effects of the inlet gas temperature and microwave power, gas velocity, bed porosity and the heat of reaction on performance of the packed bed reactors have been presented.

1. Introduction

1.1. Process intensification using microwaves

Microwave heating offers many advantages over convective heating. It is direct, volumetric and selective [1]. Moreover, microwave heating is practically instantaneous when compared to convective heating. It can also be more profitable than convective heating as shown in a previous work [2]. In conclusion, these unique features of microwave heating indicate the possibility of process intensification.

Microwave heating is direct because heat is produced just within an absorbing material, i.e., the material that has the ability to convert the microwave energy into heat, while the required electromagnetic energy is remotely supplied to the material. Clearly, it means that no heating medium such as hot gas or liquid is needed to deliver heat. Microwaves are usually generated by a magnetron. Then, they are typically transferred in the air to be finally converted into heat in the irradiated material.

Microwave heating is volumetric because it is not restricted by the heat transfer surface. Note that this limitation concerns conductive and convective heating. On the other hand, when microwaves operate, heat is produced directly in the volume of the absorbing material. Notice, however, that volumetric heating is restricted to some extend because of the characteristic distance that is accessible for microwaves. More strictly, this characteristic distance called the penetration depth is defined as the depth at which the power density decreases to 37% of its initial value at the surface. This parameter is defined as

$$D_p = \frac{\lambda_0}{2\pi\sqrt{(2\varepsilon')}} \frac{1}{\sqrt{\left(\sqrt{1+\left(\frac{\varepsilon''}{\varepsilon'}\right)^2}-1\right)}} \quad (1)$$

where λ_0 is the wavelength of microwaves, ε' is the relative permittivity (the real part of the complex permittivity $\varepsilon^* = \varepsilon' + i\varepsilon''$) which is a measure of the ability of a dielectric material to be polarized under the influence of an electric field, ε'' is the loss factor (the imaginary part of the complex permittivity $\varepsilon^* = \varepsilon' + i\varepsilon''$) which is a measure of the ability of a dielectric material to convert the absorbed energy into heat.

Microwave heating is selective because heat is only produced in a material that has appropriate dielectric properties. Precisely, the ability of the material to convert microwave energy to thermal energy is defined by the loss tangent

$$\tan\delta = \frac{\varepsilon''}{\varepsilon'} \quad (2).$$

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Nomenclature

A	pre-exponential factor, 1/s
C_{Ag}	concentration of A reactant in the gas, mol/m^3
C_{As}	concentration of A reactant in the solid, mol/m^3
c_p	specific heat capacity, J/(kg K)
D,d	diameter, m
D_L	effective axial mass dispersion, m^2/s
D_p	penetration depth of microwaves, m
D_R	radial dispersion coefficient, m^2/s
E	activation energy, J/mol
F	surface area of inlet face of the reactor, m^2
ΔH_R	enthalpy of reaction, J/mol
h	heat transfer coefficient, W/(m^2 K)
k_c	mass transfer coefficient between the gas and particles, m/s
L	length of reactor, m
$\dot{m}$	gas mass flow rate, kg/s
P_0	incident microwave power, W
P_{el}	electrical power, W
R	gas constant, J/(mol K)
$\dot{Q}_{mw}$	local volumetric power dissipation due to microwaves, W/m^3
R_A	reaction rate, mol/(m^3 s)
T	temperature, K
t	time, s
z	spatial coordinate
Y	$Y = \dot{m}_{CR}/\dot{m}_{MR}$
Pe_r	Peclet number
$Re_p = \frac{\dot{m}d_s}{F\mu}$	particle Reynolds number

Greek symbols

ϕ	bed porosity
$\hat{\varepsilon}$	intraparticle porosity
ε'	dielectric constant
ε''	dielectric loss
η	efficiency factor
λ_0	wavelength of microwave radiation, m
λ_g	molecular thermal conductivity of gas, W/(m K)
λ_{eg}	effective axial thermal conductivity in the gas, W/(m K)
λ_{es}	effective axial thermal conductivity in the particles, W/(m K)
$\lambda_{e,z}$	effective axial thermal conductivity, W/(m K)
$\lambda^o_{e,z}$	effective static axial thermal conductivity, W/(m K)
v_z	axial gas velocity, m/s
v_{rA}	stoichiometric coefficient of the A reactant
ρ	density, kg/m^3
τ	tortuosity factor for diffusion

Subscripts

0	initial, reference
a	ambient
el	electrical
el → heat	electrical energy conversion into heat
el → mw	electrical energy conversion into microwaves
g	gas
i	inner
in	inlet
mw	microwave
o	outer
out	outlet
s	solid (particles)
w	wall

The frequency dependences of ε' and ε'' are presented below

$$\varepsilon' = \varepsilon'_\infty + \frac{(\varepsilon'_0 - \varepsilon'_\infty)}{(1+\omega^2\tau^2)} \tag{3}$$

$$\varepsilon'' = \frac{(\varepsilon'_0 - \varepsilon'_\infty)\omega\tau}{(1+\omega^2\tau^2)} \tag{4}$$

where ε'_0 is the static dielectric constant, ε'_∞ is the high frequency constant, ω the angular frequency ($\omega = 2\pi f$), and τ the relaxation time defined for spherical dipoles as follows

$$\tau = \frac{4\pi r^3 \mu}{kT} \tag{5}$$

where r is a radius of the dipole, μ the dynamic viscosity, k the Boltzman's constant and T the temperature.

Table 1 presents loss tangents for a few selected materials. It follows from the data that glycerol and water have loss tangents that are remarkably greater than those of air and Teflon. This reveals that only the former materials can convert microwave energy into heat, while the latter ones are transparent for microwaves.

Microwave heating has been utilized effectively in several classes of chemical reactions. The majority of applications have been reported in organic synthesis where the enhancement due to microwaves has been displayed for the following sub-classes of chemical reactions: *N*-acylation, alkylation, aromatic and nucleophilic substitution, condensation, cycloaddition, deprotection and protection, esterification and transesterification, heterocycles, organometallic reactions, oxidation, rearrangement and reduction [3]. This subject is covered in a few extensive reviews [3–6].

Numerous applications of microwave heating have been also demonstrated in heterogeneous gas-phase catalysis [7,8]. In this case, the observed enhancements have concerned higher conversion and selectivity as well as reduction in the reaction temperature. In turn, hot-spots, selective heating, plasma formation and arcing have been indicated as the possible explanations of the reported enhancements.

Apart from the use of microwaves in various kinds of chemical reaction, microwave heating has established its position in some industrial applications. The most important ones are as follows: food tempering, pre-heating for rubber vulcanization, drying, heating and cooking, pasteurization and sterilization [8]. Besides, the potential for process intensification has been proved in the case of the following processes: extraction, distillation, crystallization, membrane separation and adsorbent regeneration [8].

1.2. Modeling of microwave-assisted heterogeneous catalysis

This work presents numerical study on heat and mass transfer in the microwave-assisted (MR) and the conventional (CR) packed bed reactors with an irreversible first-order endothermic chemical reaction.

Previous works showed that microwave heating could be especially attractive for endothermic catalytic reactions [9–12]. More detailed, heat transfer limitations occurring in the

Table 1
Loss tangents, tan δ of some selected materials.

Material	Frequency (GHz)	Loss tangent, tan δ
Air	2.45	0
Glycerol	2.45	0.54
Teflon	10	0.0004
Water (distilled)	3	0.157