Electronic Supplementary Information

A hierarchical approach to chemical reactor engineering: an application to micro packed-bed reactors

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1. Equations of Wellauer correlation

Herein the correlation for the effective radial thermal conductivity and the wall heat transfer coefficient, suggested by Wellauer et al. [23] , is reported. These equations should be applied to estimate $k_{r,eff}$ and h_W in Eq. (15). In the following equations the superscripts f and s represent the fluid and solid properties, respectively.

$$k_{r,eff} = k_r^f + \frac{k_r^s\left(1-\frac{4}{Bi^f}\right)}{\left(1-\frac{8}{N_s}\right)} \quad \text{(A.1)}$$

$$Bi^f = \frac{h_W^f D_C}{2k_r^f} \quad \text{(A.2)}$$

$$Bi^f = 5.73\left(\frac{D_C}{D_P}\right)^{1/2} \mathrm{Re}^{-0.26} \quad \text{(A.2)}$$

$$N_s = \frac{1.5(1-\varepsilon)hD_C^2}{k_r^s D_P} \tag{A.3}$$

$$k_r^f = \frac{Gc_P D_P}{8.6\left(1+19.4\left(\frac{D_P}{D_C}\right)^2\right)} \tag{A.4}$$

$$k_r^s = k_r^s\left(1+2.66\sqrt{\frac{1}{N}}\right) \tag{A.5}$$

$$k_r^s = \frac{k^f(1-\varepsilon)}{\left[\frac{2}{3A}+\phi\right]} \tag{A.6}$$

$$\phi = \phi_2 + \frac{(\phi_1-\phi_2)(\varepsilon-0.26)}{0.216} \tag{A.7}$$

$$\phi_1 = \frac{\frac{1}{3}\left(1-\frac{1}{A}\right)^2}{\ln\left(A-0.577(A-1)\right)-0.423\left(1-\frac{1}{A}\right)} - \frac{2}{3A} \tag{A.8}$$

$$\phi_2 = \frac{0.072\left(1-\frac{1}{A}\right)^2}{\ln\left(A-0.925(A-1)\right)-0.075\left(1-\frac{1}{A}\right)} - \frac{2}{3A} \tag{A.9}$$

$$A = \frac{k^s}{k^f} \tag{A.10}$$

$$h = \frac{0.574}{\varepsilon}(Gc_P)\,\mathrm{Re}^{-0.407} \tag{A.11}$$

2. Details on notation, symbols and unit of measurements

Latin letters

D_C	honeycomb channel diameter	[m]
D_P	particle diameter	[m]
c_P	gas specific heat at constant temperature	[J/kg/K]
G	specific mass flow rate	[kg/m^2/s]
h_W	wall heat transfer coefficient	[W/m^2/K]
$k_{eff,ax}$	effective axial thermal conductivity of honeycomb matrix	[W/m/K]
$k_{eff,r}$	effective radial thermal conductivity of honeycomb matrix	[W/m/K]
k	thermal conductivity	[W/m/K]
L	reactor length	[m]
N	tube-to-particle diameter ratio	[-]
Q^{REACT}	heat generated by the reaction	[W/m$^3_{cat}$]
R_i	reaction rate of the i-th species	[kg/m$^3_{cat}$/s]
R	tube radius	[m]
r	radial coordinate	[m]
S_v	exchange area between the packing and the honeycomb matrix	[1/m]
T	temperature	[K]
T_{wall}	external wall temperature	[K]
T_{cool}	coolant temperature	[K]
U	overall heat transfer coefficient	[W/m^2/K]
u	velocity	[m/s]
z	axial coordinate	[m]

Greek symbols

ε	void fraction	[-]
ρ	density	[kg/m^3]
ω_i	mass fraction of the i-th species	[-]
μ	molecular viscosity	[kg/m/s]

Superscript

G	gas phase
H	honeycomb matrix
P	micro-packing
0	inlet value

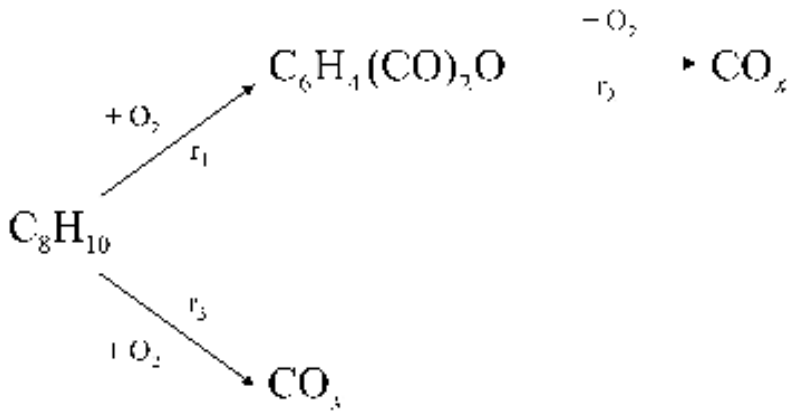
Dimensionless numbers

$\mathrm{Bi} = \dfrac{h_W D_C}{2k_{eff,r}}$ Biot number

$\mathrm{Re} = \dfrac{GD_P}{\mu}$ Reynolds number

3. Kinetic scheme

The kinetic scheme proposed by Froment et al.[2] for the selective oxidation of o-xylene to phthalic anhydride on V_2O_5 catalysts has been adopted in this work. It consists of the reactions of partial and total oxidation of o-xylene to phthalic anhydride and CO_x. Moreover, the subsequent oxidation of phthalic anhydride and CO_x is considered, as shown in Scheme S1.



Scheme S1 Reaction scheme for the selective oxidation of o-xylene to phthalic anhydride.

The reaction rates have been rederived as a function of the partial pressure of the species. The kinetic parameters are reported in Table S1.

Table S1. Reaction rate expression and kinetic constant for the selective oxidation of o-xylene to phthalic anhydride[2]

Reaction rates	Kinetic constant	
$r_1 = k_1 p_{O_2} p_{o-xy}$	$k_1 = \exp\left(-\frac{13588}{T} + 19.837\right)$	$\left[\frac{kmol\ bar^2}{kg_{cat} s}\right]$
$r_2 = k_2 p_{O_2} p_{pa}$	$k_2 = \exp\left(-\frac{15803}{T} + 20.860\right)$	$\left[\frac{kmol\ bar^2}{kg_{cat} s}\right]$
$r_3 = k_3 p_{O_2} p_{o-xy}$	$k_3 = \exp\left(-\frac{14394}{T} + 18.970\right)$	$\left[\frac{kmol\ bar^2}{kg_{cat} s}\right]$