Dehydration of 2,3-Butanediol to 1,3-Butadiene and Methyl Ethyl Ketone: Modeling, numerical analysis and validation using pilot-scale reactor data

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SUPPLEMENTARY MATERIAL

Table S1. Specification of the reactor.

	Property	Value	Unit
Catalyst	**Type**	Amorphous Calcium Phosphate (Ca/P = 1.3)	
	Average diameter	**2.855**	mm
	Weight	80	g
	Density	460.5	kg/m3
	Heat capacity [1]	995	J/(kgK)
	Conductivity	0.251	W/(mK)
	Porosity	0.121	
	Tortuosity[2-3]	1.73	
Tube	Inner diameter	30	mm
	Tube length	1195	mm
Tube wall	Thickness	3.937	mm
	Thermal conductivity	16	W/(mK)
	Heat capacity	2000	J/(kgK)
Catalyst bed	Length	378	mm
	Density	299.4	kg/m3
	Porosity	0.35	

Table S2. Reaction rate equations and kinetic parameters [4].

Reaction rate equations	$\boldsymbol{r_i = k_i C_{react,i}{}^{n_i}}$ $\boldsymbol{C_j = \frac{P_j}{RT}}$ $\boldsymbol{k_i = k_{T_{ref,i}} exp(\frac{-E_i}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right))}$		
		Unit	Value
Kinetic parameters	E_1	J/mol	2.33×10^5
	$E2$	J/mol	2.82×10^5
	$E3$	J/mol	1.93×10^5
	$E4$	J/mol	1.66×10^5
	$k_{Tref,1}$	$mol^{(1-n1)}m^{3(n1-1)}s^{-1}$	7.45×10^{-4}
	$k_{Tref,2}$	$mol^{(1-n2)}m^{3(n2-1)}s^{-1}$	4.41×10^{-4}
	$k_{Tref,3}$	$mol^{(1-n3)}m^{3(n3-1)}s^{-1}$	6.44×10^{-4}
	$k_{Tref,4}$	$mol^{(1-n4)}m^{3(n4-1)}s^{-1}$	1.27×10^{-4}
	$n1,n3,n4$	-	0.0187
	$n2$	-	0.146

Table S3. Pertinent correlations and equations for the 1D heterogeneous model .

Parameter	Formular
Mass and heat transfer coefficient between catalyst surface and fluid [5]	$Sh_p = Re_p Sc^{1/3} \max(1.66 Re_p{}^{-0.51}, 0.983 Re_p{}^{-0.41})$ $Nu_p = Re_p Pr^{1/3} \max\left(1.66 Re_p{}^{-0.51}, 0.983 Re_p{}^{-0.41}\right)$
Overall heat transfer coefficient [6]	$\frac{1}{U} = \frac{1}{h_i} + \frac{\chi_w}{\lambda_m}\frac{d_t}{\bar{d}_L}$

Tube side heat transfer coefficient [7-8]	$\frac{1}{h_i} = \frac{1}{\alpha_{ws}^e} + \frac{d_t/2}{3\lambda_{rs}^e}\frac{Bi+3}{Bi+4}$ $\alpha_{ws}^e = \alpha_{ws,0}^e + \alpha_{ws,d}^e$ $\lambda_{rs}^e = \lambda_{rs,0}^e + \lambda_{rs,d}^e$
Effective diffusivity within a catalyst [9]	$D_e = D\_mean(\varepsilon_p/\tau)$
The effectiveness factor [9]	$\eta_i = \int_0^{r_p} r_{si} dr/(r_p r_{si,s})$

Nomenclature

Bi	Biot number, m
C	mole concentration, mol/m3
$\bar{d}_L$	logarithmic mean diameter, m
d_t	diameter of a reactor, m
D_e	effective diffusivity within a catalyst, m2/s
D_mean	mean diffusivity coefficient, m2/s
E	activation energy, J/mol
h_i	tube inside heat transfer coefficient, W/m2 K
k	reaction rate constant, mol(1-*n*) m3(*n*-1) s-1
$k_{T_{ref}}$	transformed adsorption pre-exponential factor, m3/mol
n	reaction order
Nu_p	Nusselt number for fluid-solid heat transfer
P	pressure, Pa
r	reaction rate, mol/kg-cat s
r_p	catalyst radius, m
r_{si}	reaction rate in catalysts, mol/kg-cat s
$r_{si,s}$	reaction rate at the surface of the catalyst, mol/kg-cat s
R	ideal gas law constant, J/mol K
Re_p	Reynolds number for packed bed
Sc	Schmidt number
Sh_p	Sherwood number for packed bed
T	temperature, K
T_{ref}	reference temperature, K
U	overall heat transfer coefficient, W/m2 K
x_w	tube wall thickness, m

Greek letters

α_{ws}^e	effective bed-wall heat transfer coefficient, W/m2 K
$\alpha_{ws,0}^e$	static term of the effective bed-wall heat transfer coefficient, W/m2 K
$\alpha_{ws,d}^e$	dynamic term of the effective bed-wall heat transfer coefficient, W/m2 K
ε_p	catalyst porosity
η	effectiveness factor
λ_m	wall thermal conductivity, W/m K
λ_{rs}^e	effective bed heat conductivity, W/m K
$\lambda_{rs,0}^e$	static term of effective bed heat, W/m K
$\lambda_{rs,d}^e$	dynamic term of effective bed heat conductivity, W/m K
τ	catalyst tortuosity
Subscripts	
i	reaction *i*
j	species *j*
react	reactant
rxn	reaction

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