Optimization of mechanical agitation and evaluation of the mass-transfer resistance in the oil transesterification reaction for biodiesel production

Supporting Information

Evaluation of the parameters and mass-transfer coefficients contained in the expressions of the characteristic times of non-polar side and polar-side triglyceride transport ($t_{T,NP}$, $t_{T,P}$) and of triglyceride diffusion in the polar film ($t_{D,P}$).

The mass-transfer coefficient of triglyceride diffusion in the polar (dispersed) phase, $k_{TG,P}$, was evaluated according to Ahn and Lee,[38] and Kronig and Brink:[39]

$$k_{TG,P} = 17.9\frac{D_{TG,P}}{d_{32}} \tag{SI-1}$$

The diffusivities of triglycerides in the polar and non-polar phases, $D_{TG,P}$ and $D_{TG,NP}$, were evaluated according to Sinnott:[40]

$$D_{TG,P} = 1.173\cdot 10^{-13}\frac{(1.9M_{TG})^{0.5}\vartheta}{1000\mu_P V_{mol,TG}^{0.6}} \tag{SI-2}$$

$$D_{TG,NP} = 1.173\cdot 10^{-13}\frac{(1.9M_{TG})^{0.5}\vartheta}{1000\mu_{NP} V_{mol,TG}^{0.6}} \tag{SI-3}$$

$D_{TG,P}$ and $D_{TG,NP}$ resulted equal respectively to $8.2\cdot 10^{-10}$ m^2/s and $6.8\cdot 10^{-11}$ m^2/s.

The overall coefficient of triglyceride interfacial transport from the non-polar to the polar phase, $K_{TG,P}$, was estimated as:

$$\frac{1}{K_{TG,P}} = \frac{1}{k_{TG,P}} + \frac{1}{m_{TG}\cdot k_{TG,NP}} \tag{SI-4}$$

The triglyceride partition coefficient, m_{TG}, was estimated as $\rho_{TG}/s_{TG,P}$, where $s_{TG,P}$, the triglyceride solubility in methanol at 60 °C, was taken equal to 4 g/L according to Boocock et al.[36] The mass-transfer coefficient of triglyceride diffusion in the non-polar (continuous) phase, $k_{TG,NP}$, was evaluated according to the following equation, derived from the correlations reported by Hiraoka et al.:[41]

$$k_{TG,NP} = 0.45 \frac{D_{TG,NP}^{0.666} \ \rho_c^{0.053} \left(P_V\right)^{0.193}}{d_{32}^{0.228} \mu_c^{0.246}} \qquad \text{(SI-5)}$$

The evaluations of $k_{TG,NP}$ obtained with eq SI-5 are in very good agreement with those obtained following the alternative approach suggested by Skelland and Moeti.[42]

Finally a, the specific interfacial area, was evaluated as $6\ \varepsilon_P / d_{32}$.

Nomenclature relative to the Supporting Information

a	specific interfacial area referred to the total volume of the two phases (m^2/m^3)
d_{32}	Sauter mean diameter of dispersed phase droplets (m)
D	impeller diameter (m)
$D_{TG,NP}$	diffusivity of triglycerides in the non-polar phase (m^2/s)
$D_{TG,P}$	diffusivity of triglycerides in the polar phase (m^2/s)
$K_{TG,P}$	overall mass-transfer coefficient of triglyceride interfacial transport (m/s)
$k_{TG,P}$	mass-transfer coefficient of triglyceride diffusion in the polar (dispersed) phase (m/s)
$k_{TG,NP}$	mass-transfer coefficient of triglyceride diffusion in the non-polar (continuous) phase (m/s)
m_{TG}	triglyceride partition coefficient between the non-polar and the polar phase (-)
M_{TG}	average molar mass of the triglycerides (866 g/mol)
P_V	impeller power per unit reactor volume (W/m^3)
$s_{TG,P}$	triglyceride solubility in methanol at 60 °C (4 kg/m^3)
$V_{mol,TG}$	molar volume of the triglycerides (m^3/kmol)
ε_P	volume fraction of the polar (dispersed) phase (-)
μ_c	viscosity of the continuous phase (Pa s)

μ_{NP}	viscosity of the non-polar phase (Pa s)
μ_P	viscosity of the polar phase (Pa s)
ρ_c	density of the continuous phase (kg/m^3)
ρ_{TG}	density of the triglycerides (kg/m^3)
θ	temperature (K)