Esterification & Transesterification reactions play a key role in today’s biorefineries. Conventionally, these reactions are performed using an acid or a base homogeneous catalyst. Heterogeneous catalysis (+) not dedicated catalyst separation (+) no purification.

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Introduction & scope

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Esterification

Reaction Mechanism & Kinetic model

Chemical equilibrium

\[
\text{MeOAc} + \text{H}^+ \rightleftharpoons \text{MeOH} + \text{Ac}^+ \\
\text{SR} + \text{Ac}^+ \rightleftharpoons \text{SR}_{\text{Ac}}^+ \\
\text{MeOAc} + \text{SR}_{\text{Ac}}^+ \rightleftharpoons \text{MeOH} + \text{AcAc}
\]

Kinetic rate law

\[
\text{k}_\text{obs} = \frac{1}{\text{t}} \cdot \ln \left( \frac{C_{\text{MeOAc}}}{C_{\text{MeOAc}}^0} \right) = \frac{1}{\text{t}} \cdot \ln \left( \frac{C_{\text{MeOH}}}{C_{\text{MeOH}}^0} + 1 \right)
\]

Catalyst

Lewatit K1221

No permanent pore structure
Pore structure obtained by swelling
Micropores
4 % DVB

Modelling results

\[
\begin{align*}
\text{k}_{\text{obs}} &= (10^{-3} \text{ mol kg}^{-1} \text{s}^{-1}) \\
50.8 \pm 6.0 &= 52.7 \pm 0.3 \\
E &= (46.1 \pm 1.9) \text{ KJ mol}^{-1} \\
4.3 \pm 0.3 &= 1.2 \pm 0.1 \\
0.0 &= 4.9 \pm 0.4 \\
7.9 \pm 0.7 &= 100
\end{align*}
\]

Conclusions & perspectives

- Temperature and initial molar ratio effect adequately modelled with proposed reaction mechanism.
- In the mechanism are all the acid sites covered and is sorption expressed by an exchange.
- Activation energy of 48 KJ mol\(^{-1}\), irrespective of the reaction type.
- Unique set of exchange coefficients for each reaction.
- High value of ion-exchange coefficient \(K_w\) shows the inhibiting effect of water on the esterification.
- For 333 K and initial molar ratio of 10:1, at least 60 % of the catalyst’s active sites were covered by methanol.

Acknowledgements

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