3D Simulation of Fatty Acid Methyl Ester Production in a Packed Membrane Reactor

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Introduction:

The current work is aimed to simulate the production of high quality biodiesel from palm oil in a micro porous ceramic membrane reactor. The TiO_2/Al_2O_3 ceramic membrane was used as the separator and catalytic bed. It was packed with potassium hydroxide catalyst supported on palm shell activated carbon.



Results:

Investigation of velocity is the best suggestion for finding the optimum value of the components' residence time and reactor length. In our case we found that the residence time is not matched with the reactor length and it affected the reaction efficiency



Figure 3. Contours of velocity magnitude (m/sec) within the catalytic bed and ceramic membrane

Figure 4. Velocity vectors within the module at steady state condition

CFD results were indicated that increasing the reaction temperature leads to

Figure 1. A schematic diagram of biodiesel production

The investigation of components distribution within the system was not possible. Hence CFD analysis was used to predict the distribution of biodiesel and the other by-products in the membrane module.



Figure. 2. A schematic diagram of micro porous ceramic membrane reactor

Computational Methods:

The flow field was obtained by solving the continuity equation and the momentum balance equations of the system.

 $\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial(\rho\vec{v}\varepsilon)}{div(\rho\vec{u}\varepsilon)} = \frac{DiffusionTerm}{div(\Gamma_{\varepsilon}grad\varepsilon)} + S_{\phi}^{sourceTerm}$

the same conversion in shorter time, or increase in temperature by 10°C, results in 5 % growth of reaction for the same time period.





Figure 5. Concentration distribution (mol/m³) within the catalytic bed at different times and temperature of 60 °C.

The molar concentrations of each component are also shown in the total system for 85 sec and 400 sec.



Figure 7. Concentration distribution of different components (mol/m³) within the catalytic bed and ceramic membrane.

Conclusions

The Brinkman equation was used to simulate fluid flow within the porous media.

 $div\,\sigma^d - \nabla p - c\vec{u} = 0$

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In addition, the Maxwell-Stefan equation was applied for simulation of reaction kinetics and mass transfer.

$$\nabla \cdot \left[\rho \omega_i u - \rho \omega_i \sum_{j=1}^n \widetilde{D}_{ij} \left(\nabla x_j + \left(x_j - \omega_j \right) \frac{\nabla p}{p} \right) - D_i^T \frac{\nabla T}{T} \right] = R_i$$

The combination of mentioned models was solved mathematically by means of the finite element method and PARDISO algorithm.

- A catalytic bed ceramic membrane was employed for biodiesel production.
- The system was a combination of the reaction/separation inside one single shell.
- Using CFD simulation we found that the residence time is not matched with the reactor length and it affected the reaction efficiency.
- Analysing the diffusion parameter, shows that at the area near and within the ceramic membrane wall, diffusion is more prominent.
- While at the middle section, the convection term is more applicable for all components.

References

[1] B. Sajjadi, A.R. Abdul Aziz, S. Baroutian, S. Ibrahim, Investigation of convection and diffusion during biodiesel production in packed membrane reactor using 3D simulation, J Ind Eng Chem, 20 (2014) 1493-1504.



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