Investigation of convection and diffusion during biodiesel production in packed membrane reactor using 3D simulation
1. University of Malaya, Department of Chemical Engineering
2. University of Malaya, Department of Civil Engineering
50603 Kuala Lumpur, MALAYSIA.

Introduction: This work exhibits the simulated convection and diffusion phenomena in a TiO$_2$/Al$_2$O$_3$ membrane reactor during transesterification for biodiesel production.

Computational Methods: The reactor is symmetrical so only half of the system was simulated. The continuity and momentum balance equation is expressed by:

$$\frac{\partial (\rho \vec{e})}{\partial t} = - \text{div}(\rho \vec{u} \vec{e}) + \text{div} \left( \Gamma \frac{\partial \vec{e}}{\partial x} \right) + S_\phi$$

Brinkman equation describes fluid flow in porous bed as modification to the Navier-Stokes equation:

$$\mu \nabla^2 \vec{u} - \nabla p - \frac{\mu}{k_{hr}} \vec{u} = 0$$

The Maxwell-Stefan diffusion and convection equations at steady state serve as mass-balance equations in the catalytic bed:

$$\frac{\partial c_i}{\partial r} + \nabla \left( - D_i \left( \frac{\partial c_i}{\partial x} + \frac{\partial c_i}{\partial y} + \frac{\partial c_i}{\partial z} \right) \right) + u_i \left( \frac{\partial c_i}{\partial x} + \frac{\partial c_i}{\partial y} + \frac{\partial c_i}{\partial z} \right) + \beta c_i = R_i$$

$$N_i = -D_i \left( \frac{\partial c_i}{\partial x} + \frac{\partial c_i}{\partial y} + \frac{\partial c_i}{\partial z} \right) + u_i c_i$$

$$\nabla \left[ \rho \omega_i u - \rho \omega_i \sum_j D_j \left( \nabla x_j + (x_j - \omega_j) \frac{\nabla p}{p} \right) - D_j \frac{\nabla T}{T} \right] = R_i$$

Results:

Figure 1. Boundary conditions at different surfaces of the membrane reactor

Conclusions: This work enables us to visualise and analyse the convective and diffusive process inside the membrane reactor.

References: