MATERIALS AND METHODS

Theoretically, the reactive distillation process requires the experiment data for design and construction. In order to reduce tradition work and time, the simulation can be served this design information. In this research, the simulations were carried out by the industrial simulation package named ASPEN PLUS 2004.1.

The objective is to compare two processes of Jatropha biodiesel productions (conventional and reactive distillation processes). In general, combination of reaction and separation to one unit is more difficult to control than the conventional distillation. This reactive distillation processes give nonlinear characteristics such as multiple steady states and high sensitivity to operating. Therefore, the ASPEN DYNAMICS is used to study the dynamics behavior on the reactive distillation of biodiesel production.

1. Process description

The production of biodiesel by alkali catalyst transesterification was simulatedby Zhang (Zhang *et al*., 2003). There are consists of 6 processes as shown in the Figure 10.

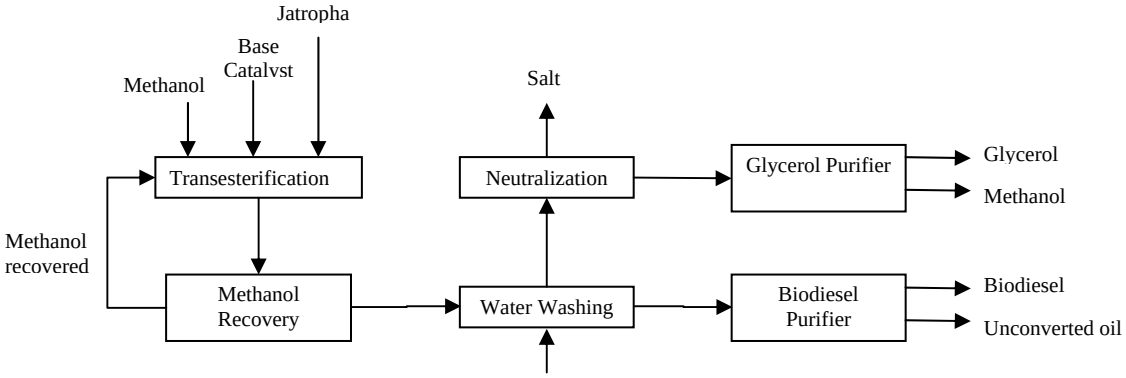


Figure 10 Process facilities of biodiesel process

The details of each process are described below.

1. Transesterification section; the Jatropha reacts with methanol and catalyst.
2. Methanol recovery section; the excess of methanol are separated and recycled.
3. Water washing section; the NaOH is diluted by water.
4. Biodiesel purifier section; the unconverted oil is separated.
5. Alkali removal section; the NaOH is neutralized.

6. Glycerol purification section; glycerol is refined as sold able grade (more than 80% or 93%).

However, the biodiesel and glycerol are not soluble together (Zhou *et al*., 2006). The solubility of multi components that consists of FAME, methanol, oil and glycerol were illustrated by phase diagram. As a result, FAME and glycerol can slightly dissolve. After the transesterification reaction complete, there are two layers which are FAME and glycerol layers. Therefore, after recovery methanol section, the FAME and glycerol should be separated. Then, the modification biodiesel process can be seen in the Figure 11.

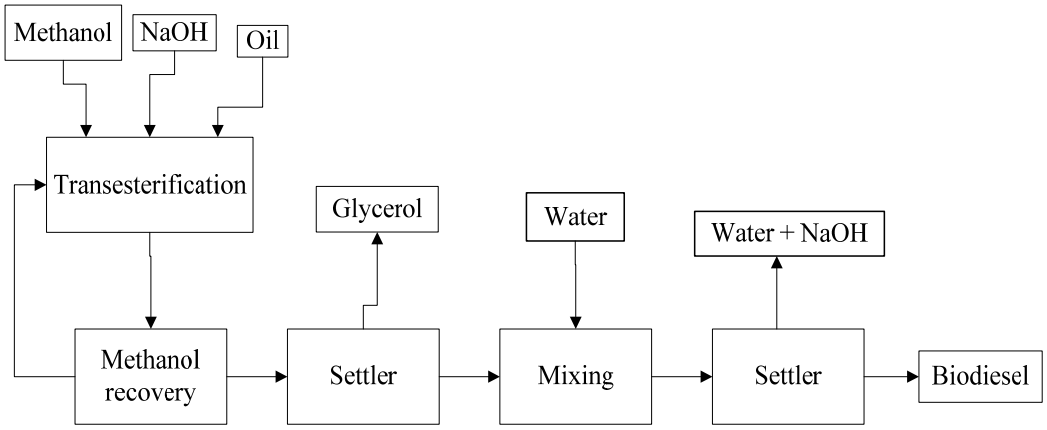
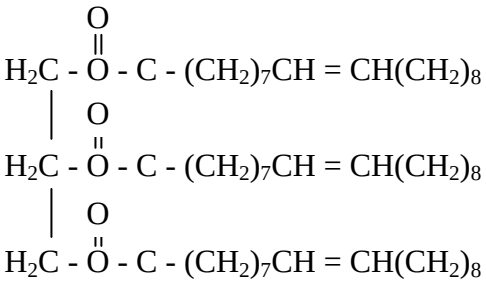


Figure 11 The modification biodiesel process from Zhang

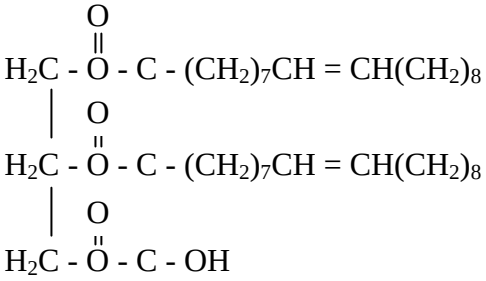
2. Steady state simulation

The simulation procedures involves defining chemical components, selecting a thermodynamics property, determining plant capacity, choosing proper operating units and setting up input conditions (flowrate, temperature, pressure and other conditions). Many components such as methanol, sodium hydroxide and glycerol are available from the library of ASPEN PLUS. The trioleic and trilinoleic acid are major component of Jatropha oil (Chatakanonda *et al*., 2005) while methyl oleate and methyl linoleate are biodiesel. All of this structure cannot obtain from ASPEN PLUS library. Therefore, the unavailable components such as mono, di, tri and methyl oleate of oleic acid and linoleic acid demonstrated in the Figures 12 and 13 are defined by GaussViewW. The proposed structures were optimized by GAUSSIAN 03W for the most stable structure. These structures were import to ASPEN PLUS in the mol format to fulfill the simulation data. The

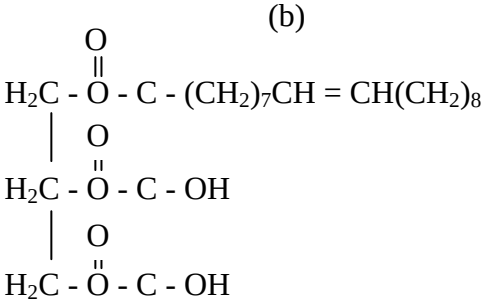
other technique for defining the unavailable structure is adding the structure in the ASPEN PLUS shown in the appendix F. Due to the methanol and glycerol are highly polar components, the non-random two liquid (NRTL) thermodynamic/activity models was recommend to predict the activity coefficients of the components in the liquid phase.



(a)



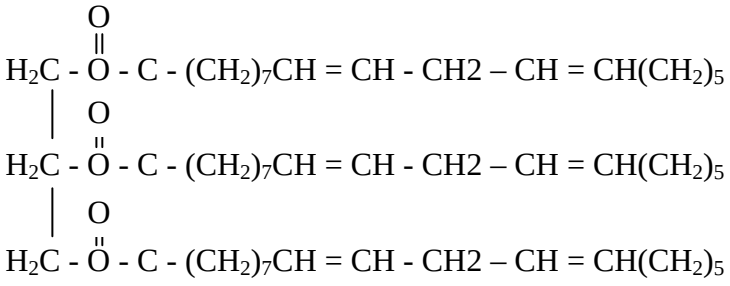
(b)



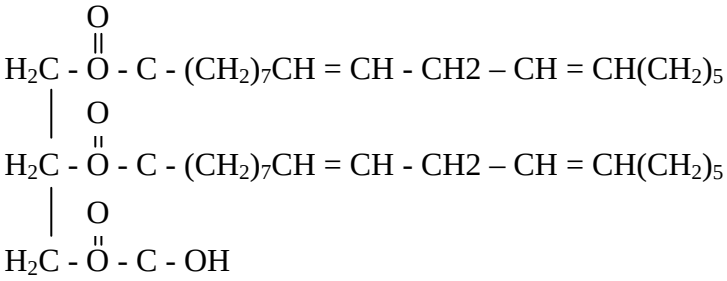
(c)

(d)

Figure 12 (a) Trioleic structure (b) Dioleic structure (c) Monooleic structure (d) Methyl oleic structure



(a)



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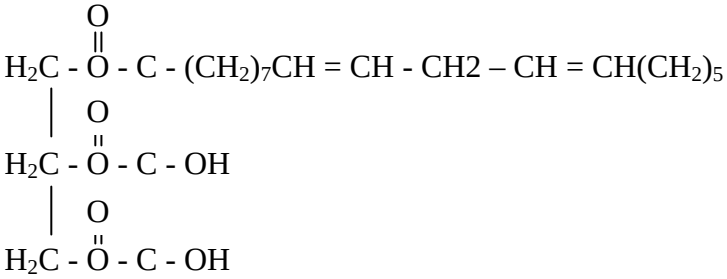

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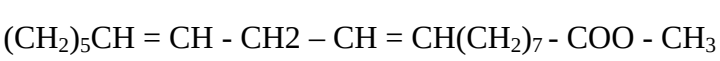

(d)

Figure 13 (a) Trilinoleic structure (b) Dilinoleic structure (c) Monolinoleic structure (d) Methyl linoleic structure

3. Dynamic simulation

The dynamic simulations are carried out by ASPEN DYNAMICS. The procedure starts with adding the value between streams and the necessary equipment data in the steady state simulation. The process is then export to ASPEN DYNAMICS which feed oil is changed as step input for studying the controllability of process.