Combination of Reactor System for Methyl Ester Fabrication

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Abstract

The main purpose of this learning is to establish the reactor configurations for biodiesel fabrication through achievable region technique. The systematic design technique is basically used for influential reactor configurations that will fabricate the optimal creation. Kinetic model for biodiesel invention was urbanized for Plug-Flow Reactor, PFR and permanent Stirred-Tank Reactor, CSTR. The representation was solved in MATLAB and consequently applied in the achievable region method to conclude the reactor structure of two different biodiesel feedstock; waste sunflower oil and rapeseed oil. The results indicate that a CSTR is an optimal reactor with maximum conversion of triglyceride. The synthesis of reactor network in chemical production can be carried out by using a graphical scheme or by superstructure optimization approaches.

Keywords: *Attainable region, biodiesel, kinetic, reactor.*

I. INTRODUCTION

The plug flow reactor reproduction is a model used to illustrate chemical reactions in uninterrupted, graceful systems of cylindrical geometry. The PFR model is worn to predict the performance of chemical reactors of such propose, so that key reactor variables, such as the proportions of the reactor, can be predictable. The key supposition is that as a plug flows throughout a PFR, the fluid is completely mixed in the radial trend but not in the axial course. Each plug of discrepancy volume is measured as a separate individual, successfully an infinitesimally small continuous stirred tank reactor, preventive to zero quantity.

In the simplest case of a PFR representation, several key assumptions must be completed in order to make simpler the problem, some of which are outlined underneath. Communication that not all of these assumptions are compulsory; nevertheless the removal of these assumptions does augment the difficulty of the predicament. The PFR model can be used to model numerous reactions as well as reactions concerning changing temperatures, pressures and densities of the flow. Even though these complications are unobserved in what follows, they are often applicable to manufacturing processes.

One of the most important steps after improvement and purpose of the structure of a chemical system and the kinetics is to find a suitable reactor which promises a complete process. The synthesis of reactor network in chemical production can be carried out by using a graphical scheme or by superstructure optimization approaches. This efficient design production method is called achievable region technique and was originated by Horn (1964). This technique determines the area of accessibility involves in numerous steps such as assortment of fundamental processes, define and vector drawing development, construction the region, understand the boundaries and discover the most favorable value.

For biodiesel production, the overall reaction is:

$$TG + 3CH_3OH \xrightarrow{\text{Catalyst}} 3RCOOH_3 + GL \quad (1)$$

The stepwise reaction that occurs during the reaction process is listed as follow:

$$TG + CH_3OH \underset{K_{-1}}{\overset{K_{+1}}{\rightleftharpoons}} R_1COOH_3 + DG \quad (2)$$

$$DG + CH_3OH \underset{K_{-2}}{\overset{K_{+2}}{\rightleftharpoons}} R_2COOH_3 + MG \quad (3)$$

$$MG + CH_3OH \underset{K_{-3}}{\overset{K_{+3}}{\rightleftharpoons}} R_3COOH_3 + GL \quad (4)$$

Where *TG*, *DG*, *MG*, *GL*, $RCOOH_3$, CH_3OH and k_i are triglyceride, di glyceride, mono glyceride, glycerol, ester, methanol, and response rate constants of each reaction, correspondingly. This paper aims to establish the reactor constitution that yields the optimal methyl esters resultant from two dissimilar feed stocks by achievable region technique.

II. METHODOLOGY

A. *Attainable Region Method*

To examine the path of a plug flow reactor (PFR) with a changeable habitation time and a fixed triglyceride's feed and methyl ester's feed the subsequent ordinary discrepancy equations have to be solved from the feed position.

$$-\frac{dC_T}{dt} = k_{+1}C_T C_A - k_{-1}C_D C_{E1} \quad (5)$$

$$-\frac{dC_D}{dt} = -\left(k_{+1}C_T C_A - k_{-1}C_D C_{E1} - k_{+2}C_D C_A + k_{-2}C_M C_{E2}\right) \quad (6)$$

$$-\frac{dC_M}{dt} = -\left(k_{+2}C_D C_A - k_{-2}C_M C_{E2} - k_{+3}C_M C_A + k_{-3}C_G C_{E3}\right) \quad (7)$$

$$-\frac{dC_{E1}}{dt} = -\left(k_{+1}C_T C_A - k_{-1}C_D C_{E1}\right) \quad (8)$$

$$-\frac{dC_{E2}}{dt} = -\left(k_{+2}C_D C_A - k_{-2}C_M C_{E2}\right) \quad (9)$$

$$-\frac{dC_{E3}}{dt} = -\left(k_{+3}C_M C_A - k_{-3}C_G C_{E3}\right) \quad (10)$$

$$-\frac{dC_A}{dt} = k_{+1}C_T C_A - k_{-1}C_D C_{E1} + k_{+2}C_D C_A - k_{-2}C_M C_{E2} + k_{+3}C_M C_A - k_{-3}C_G C_{E3} \quad (11)$$

$$-\frac{dC_G}{dt} = -\left(k_{+3}C_M C_A - k_{-3}C_G C_{E3}\right) \quad (12)$$

Where C_T, C_A, C_D, C_M, C_{E1}, C_{E2}, C_{E3}, C_G are the concentration of triglyceride, methanol, di glyceride, monoglyceride, methyl ester 1, methyl ester 2, methyl ester 3 and glycerol, correspondingly. Published response rate constants (k_{+1} – k_{-3}) are scheduled in Table I.

Table I: Reaction Rate Constants

Reaction rate constants (l/mol. min)	Waste Sunflower Oil	Rapeseed Oil
K_{+1}	0.0772	0.0879
K_{-1}	0.1680	0.4777
K_{+2}	0.0972	0.1555
K_{-2}	0.0265	0.1396
K_{+3}	0.0670	0.7478
K_{-3}	0.0088	0.0061

Equations (6) to (12) is solved numerically with a 4th order Runge-Kutta algorithm, which is accessible in MATLAB. The explanation generates the molar concentrations of all species, *Ci*, as functions of the intend variables, i.e. the conversion of the restrictive reactant, TG, and the molar ratio of the overload methanol, A. The reasonable region for the biodiesel reaction is constructed by first machinations a PFR trajectory from the feed point, enduring to the absolute conversion of triglyceride, which is the plot of attentiveness of the main invention, methyl ester against concentration of the restrictive reactant, TG, obtained from the explanation of Equations (6) to (12). A candidate possible region is found every time the PFR plot fashioned a convex region. In adding together, a straight line representing the mixing of product and feed is drawn to fill the non-convex parts of the trajectory. A CSTR trajectory is then constructed to see if the region can be comprehensive. To construct the trajectory, the kinetic replica of CSTR needs to be solved first.

The kinetic model for uninterrupted stirred tank reactor (CSTR) is undemanding. The stoichiometric mole balance of each variety in a CSTR using the reaction kinetics in Equation (2) to (4) yields a set of non-linear equations in Equations (13) to (20).

$$C_{To} - C_T = \frac{V}{F_T}\left(k_{+1}C_T C_A - k_{-1}C_D C_{E1}\right) = \tau\left(k_{+1}C_T C_A - k_{-1}C_D C_{E1}\right) \quad (13)$$

$$C_{Do} - C_D = -\tau\left(k_{+1}C_T C_A - k_{-1}C_D C_{E1} - k_{+2}C_D C_A + k_{-2}C_M C_{E2}\right) \quad (14)$$

$$C_{Mo} - C_M = -\tau\left(k_{+2}C_D C_A - k_{-2}C_M C_{E2} - k_{+3}C_M C_A + k_{-3}C_G C_{E3}\right) \quad (15)$$

$$C_{E1o} - C_{E1} = -\tau\left(k_{+1}C_T C_A - k_{-1}C_D C_{E1}\right) \quad (16)$$

$$C_{E2o} - C_{E2} = -\tau\left(k_{+2}C_D C_A - k_{-2}C_M C_{E2}\right) \quad (17)$$

$$C_{E3o} - C_{E3} = -\tau\left(k_{+3}C_M C_A - k_{-3}C_G C_{E3}\right) \quad (18)$$

$$C_{Ao} - C_A = \tau\begin{pmatrix} k_{+1}C_T C_A - k_{-1}C_D C_{E1} + k_{+2}C_D C_A - k_{-2}C_M C_{E2} + \\ k_{+3}C_M C_A - k_{-3}C_G C_{E3} \end{pmatrix} \quad (19)$$

$$C_{Go} - C_G = -\tau\left(k_{+3}C_M C_A - k_{-3}C_G C_{E3}\right) \quad (20)$$

Another time, CSTR multiple NLE (13) to (20) is solved numerically using MATLAB. The explanation generates the molar concentrations of all variety, C_i, as functions of the intend variables, i.e. the conversion of the preventive reactant, TG, and the molar ratio of the overload inconsistent, A. The plot of the attentiveness of ME touching the adaptation or the concentration of the restrictive reactant, TG forms the CSTR trajectory. Consequently, the trajectory is checkered to see if the achievable region can be absolute. Additionally, a linear arc is plotted on the CSTR trajectory to make sure it remainder convex. A supplementary PFR trajectory is drawn from the point where the incorporation line meets the CSTR trajectory to additional expand the attainable region. The same practice was carried out for formative the appropriate reactor for the fabrication of biodiesel from waste sunflower oil and rapeseed oil.

III. RESULTS AND DISCUSSIONS

Figure 1 shows the consequence of attainable region plot of PFR obtained from dissipate sunflower oil. The plot shows non-convex part, consequently a directly line AEB that represents an incorporation line is desirable to fill the non-convex parts of the trajectory. This forms the applicant possible region. By evaluating the rate vectors (r_T/r_E) alongside the line, it is established that there are rate vectors at point E that point out of the contender possible region. These findings recommend that a supplementary CSTR trajectory is necessary.

The CSTR trajectory was drawn preparatory from the point of the convex hull that extends the constituency the majority. In this case, it is the feed point. From Figure 2, it was noted that the CSTR trajectory also forms a non-convex region thus requires a line subdivision AC to fill the non-convex segment. At point C, it is apparent that the CSTR trajectory has reached the symmetry. The result from the possible region plot has discovered that two different reactor structures untruthful on the manageable region border. The line fragment AC represents a CSTR with bypass and point C represents a CSTR.

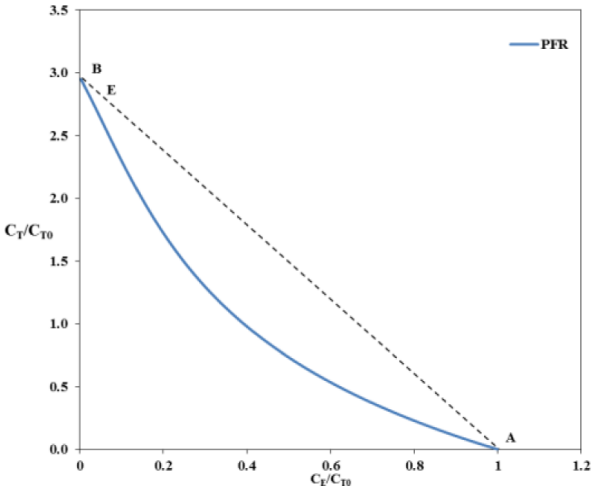

Fig. 1. Initial PFR Profile with Convex Hull for Waste Sunflower Oil.

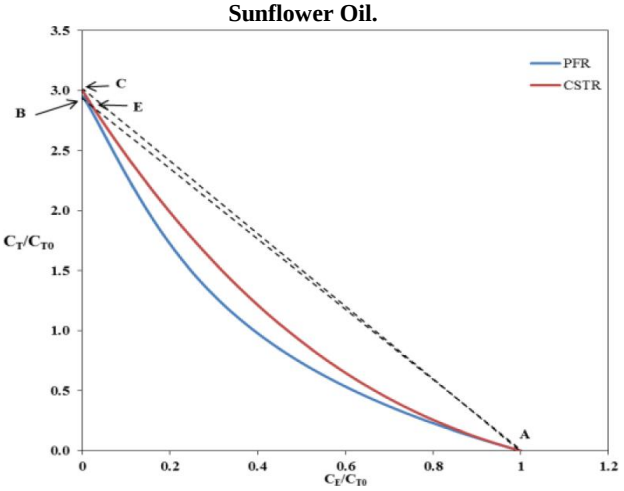

Fig. 2. PFR And CSTR Profiles With Convex Hull for Waste Sunflower Oil.

Fig. 3 presents the PFR profiles obtained from reasonable region plot of methyl ester derived from rapeseed oil. The plot also had exposed a non-convex region of PFR trajectory. Consequently, a straight line AEB was drawn to fill the non-convex parts of the trajectory thus constitutes a contender of reasonable region. The CSTR trajectory was strained from the feed point generates Figure 4. As configured in the graph, the CSTR trajectory also forms a non-convex province thus requires a line fragment AC to fill the non-convex portion. Another time, the CSTR trajectory has reached the stability at point C. The result from the reasonable region plot of biodiesel from rapeseed oil has shown

that two unusual reactor structures lying on the possible region boundary. Conversely, for waste oil, an additional esterification reactor is necessary for dropping the free fatty acid level satisfied.

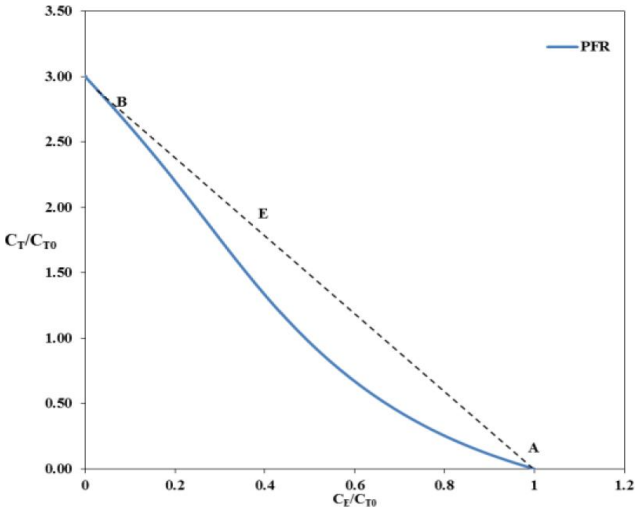

Fig. 3. Initial PFR Profile With Convex Hull for Rapeseed Oil.

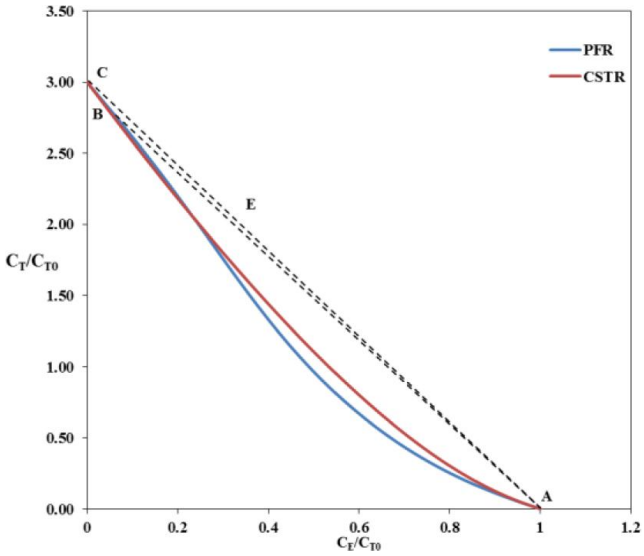

Fig. 4. PFR And CSTR Profiles and Convex Hull for Rapeseed Oil.

IV. CONCLUSION

The current revise was approved away to determine the reactor agreement of methyl ester manufacture consequent from two dissimilar types of feedstock. Possible region technique has provided an occurrence to consider unusual reactor types in order to fabricate a maximum adaptation of methyl ester by plotting the reactor trajectories. Both type of biodiesel investigated has revealed that a CSTR is an ideal reactor that can be measured for assortment. This technique determines the area of accessibility involves in numerous steps such as assortment of fundamental processes, define and vector drawing development, construction the region, understand the boundaries and discover the most favorable value.

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