A Partial Differential Equations Model Predictive Control of Heterogeneous Transesterification Process for Biodiesel Production in Tubular Reactor

Nuttanit Montriwasuwat, Paisan Kittisupakorn, Veerayut Lersbamrungsuk

Abstract - This research presents the implementation of a dynamic optimization strategy in transesterification via tubular reactor process to determine an optimal operating concentration policy maximizing concentration of biodiesel product to a product quality constraint, i.e., the requirement of coefficient of variation. Instead of assuming the perfect tracking of the optimal concentration profile, a nonlinear model predictive control (MPC) is applied to track the obtained optimal concentration policy. As feedback information of states at each time step is required in the MPC algorithm. A first-order finite difference approximation was used for this simulation. The partial derivatives in z-direction are solved to ordinary differential equations (ODEs) by the method of lines (MOL). The result of numerical integration can be optimized by using MATLAB. The manipulated variable is flow rate of cooling water. The optimization study obtains that these set points of reactor's temperature can be calculated and controlled in a sufficiently performance. The operating cost is reduced with the less IAE and higher robustness. This control can be developed for an economic reduction for the future industry of biodiesel.

Keywords: *Biodiesel; Heterogeneous catalysis; Transesterification; Model predictive control*

1. Introduction

Nowadays energy is more valuable and more required in many fields, especially in fuel energy. Fuel energy becomes more expensive and runs out quickly. Renewable energy is also an interesting alternative solution for this problem.

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Biodiesel is a renewable energy that is a production from transesterification of triglycerides. This process commonly uses homogeneous basic catalysts which need catalyst recovery or aqueous treatment steps. This paper obtains a new continuous biodiesel production process that uses heterogeneous transesterification reaction for this biodiesel production.

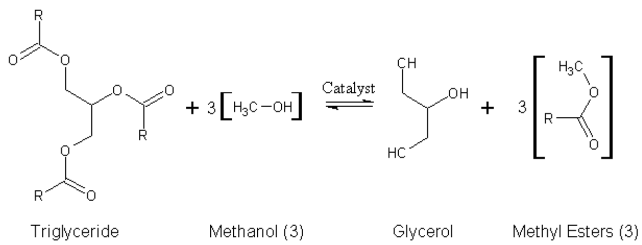

Fig.1 Transesterification reaction

The transesterification of triglycerides to fatty to fatty acid esters with methanol is balanced and show as Fig. 1. Acid or base catalyst can be used in biodiesel production. Most processes normally use homogeneous base catalysts because of faster reaction and mild reaction temperature.

However, these catalysts need to be separated from the products after the reaction step and can't be reusability catalysts. Heterogeneous solid catalysts have an important role for biodiesel production recently.

Many researches promote this heterogeneous transesterification without catalyst loss at high temperature and high pressure. Zirconium oxide (ZrO_2) was chosen with sodium hydroxide (NaOH) as a support catalyst because their physical properties were investigated by N. Abdoulmoumine[1] as a suitable economic production cost and better performance of all level of treatment than other catalysts

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2. Objective

The objective of this research is to design a MPC, a model predictive control, for a tubular reactor to track an optimal operating condition in biodiesel production and study the dynamic behavior of transesterification via heterogeneous solid catalyst

3. Modeling and simulation of the tubular reactor

MATLAB was used to conduct the simulation for the open loop behavior of transesterification and developed MPC for the control of the PDEs system. Tubular reactor is selected for the research because it takes a high conversion per unit volume for the process and easily observes the dynamic behavior in discrete distance and time

a. Component balances

The expression of the Concentration of reactant in tubular reactor is base on mole balance. The specie balances for the reactants are

$$\Delta V\frac{\partial C_A}{\partial t}=[vA_{cross}C_A]_z-[vA_{cross}C_A]_{z+\Delta z}+[A_{cross}J_A]_z-[A_{cross}J_A]_{z+\Delta z}-\Delta V\cdot rate$$

(Eq.1)

$$\Delta V\frac{\partial C_B}{\partial t}=[vA_{cross}C_B]_z-[vA_{cross}C_B]_{z+\Delta z}+[A_{cross}J_B]_z-[A_{cross}J_B]_{z+\Delta z}-3\Delta V\cdot rate$$

(Eq.2)

where J_i is molar flux of component i in the axial direction at position z

$$J_i=-D\frac{\partial C_i}{\partial z}$$

(Eq.3)

$$\frac{\partial C_A}{\partial t}=-v\frac{\partial C_A}{\partial z}+D\frac{\partial^2 C_A}{\partial z^2}-rate$$

(Eq.4)

$$\frac{\partial C_B}{\partial t}=-v\frac{\partial C_B}{\partial z}+D\frac{\partial^2 C_B}{\partial z^2}-3\cdot rate$$

(Eq.5)

b. Energy balances

The energy balance for a plug flow reactor can be derived in an analogous manner. We again perform a balance over a differential element[2].

$$\frac{\partial H}{\partial t}=-v\frac{\partial H}{\partial z}+\frac{\partial q}{\partial z}+\Delta H_r\cdot rate+\frac{Q}{V_r}$$

(Eq.6)

where q is heat flux to the temperature gradient, with the proportionality constant being, k_c, the thermal conductivity

$$q=-k_c\frac{\partial T}{\partial z}$$

(Eq.7)

Heat can also be lost through the reactor walls due to poor insulation or intentional cooling/heating in this form[4]

$$Q=A_{surf}h(T_{surf}-T)$$

(Eq.8)

$$\frac{\partial H}{\partial t}=-v\frac{\partial H}{\partial z}+k_c\frac{\partial^2 T}{\partial z^2}+\frac{A_{surf}h(T_{surf}-T)}{V_r}+\Delta H_r\cdot rate$$

(Eq.9)

$$;\frac{\partial H}{\partial t}=\frac{\partial\sum_{i=1}^{n}C_iC_{p,i}(T-T_{ref})}{\partial t}$$

$$=(T-T_{ref})\sum_{i=1}^{n}C_{p,i}\frac{\partial C_i}{\partial t}+\frac{\partial T}{\partial t}\sum_{i=1}^{n}C_iC_{p,i}$$

$$;\frac{\partial H}{\partial z}=\frac{\partial\sum_{i=1}^{n}C_iC_{p,i}(T-T_{ref})}{\partial z}$$

$$=(T-T_{ref})\sum_{i=1}^{n}C_{p,i}\frac{\partial C_i}{\partial z}+\frac{\partial T}{\partial z}\sum_{i=1}^{n}C_iC_{p,i}$$

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c. Kinetics of soybean oil transesterification

According to vegetable oil characterization (soybean oil) and catalyst characterization (1.5 M NaOH/ZrO_2-600°C), the kinetics were investigated at 60°C, 88°C and 98°C. Overall reaction order was determined a first order with respect to triglyceride and a second order with respect to methano l[1]. The activation energy and pre-exponential factor were both determined to 49.35 kJ/mol and 6.43×10^9 $M^{-1}min^{-1}$.

4. Results and discussion

In all tubular reactors, the inlet temperature plays a significant role in the design of the reactor system[5]. Higher inlet temperatures result in small reactors for the same per-pass conversion, but also result in higher exit temperatures[6].

The design of tubular reactor systems is dominated by the classical tradeoff between reactor size and flow rate velocity. Gas phase systems are particularly affected because of high cost of compression.

Simulation results with different time and distance are show the dynamic behavior of concentration of reactant, concentration of biodiesel product (fatty acid), and temperature of reactor in transesterification via heterogeneous solid catalyst in Fig.2, Fig.3 and Fig.4 respectively.

5. Control Study

A model-based feedback controller known as a model predictive control (MPC) has been found to be a successful control strategy in several industrial applications because of its ability to handle nonlinear processes, multivariable interactions, constraints, and optimization requirements[7]. For a continuous tubular reactor process, normally, a key control objective is to stabilize the system at a specified condition. In the presence of constraints on the manipulated input variables, the performance of the controlled system is limited to the conditions which stabilization can be achieved.

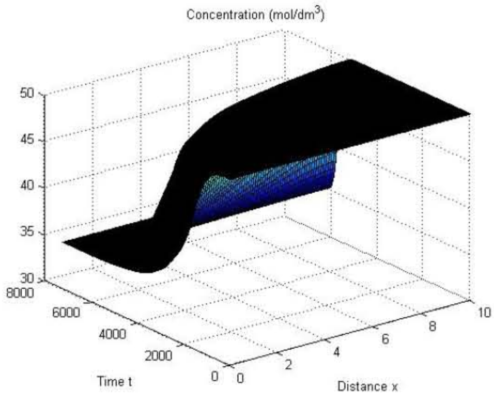

Fig.2 Concentration of methanol

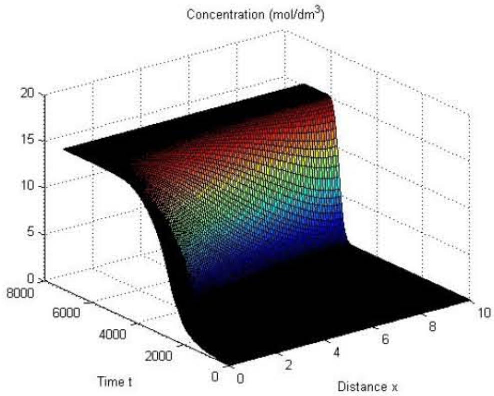

Fig.3 Concentration of fatty acid in tubular reactor

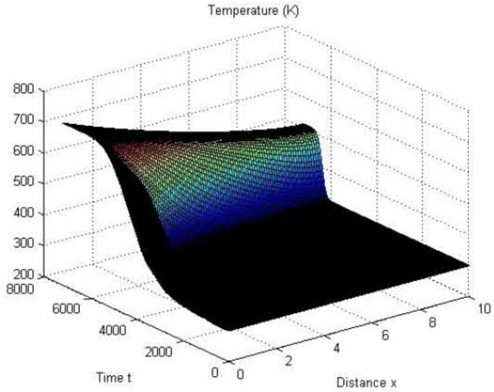

Fig.4 Dynamic behavior of temperature in tubular reactor

The purpose of this study is to design the model predictive control for a tubular reactor process, which is PDEs system, to track the T_r set point. A steam flow rate is used to control the temperature of reactor at its desired trajectory.

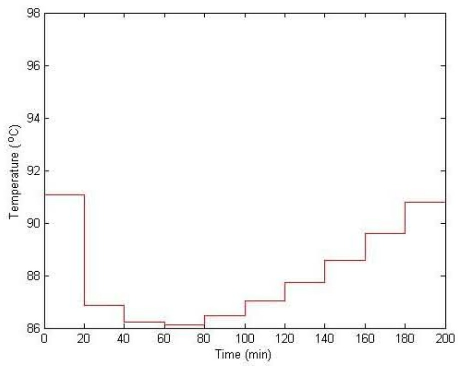

Fig.6 Optimization of transesterification in tubular reactor

In order to control the tubular reactor with MPC, the PDEs were modified by using a first-order finite difference approximation. The partial derivatives in z-direction are solved to ordinary differential equations (ODEs) by the method of lines (MOL). The result of numerical integration can be optimized by using MATLAB. The manipulated variable is flow rate of cooling water. The optimization study obtains that these set points of reactor's temperature can be calculated for the objective function with state variables and manipulated variable constraints. The

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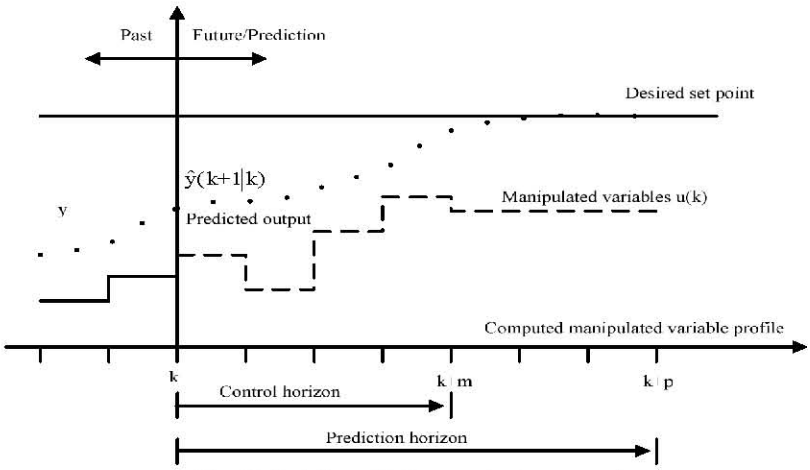

Fig.5 Model predictive control approach

results show a sufficiently performance and challenge to develop the MPC in PDEs system. The results demonstrate that robustness of the control can be improved by using MPC control integrated with the EKF for estimating unmeasurable states and uncertain parameters or other mismatch cases in the future.

6. Conclusion

A model predictive control (MPC) incorporated well with PDEs system. The designs give a good accuracy of simulation. The aim is to maximize the concentration of biodiesel product that affects the constant time of reaction and temperature. Since the MPC is a model-based controller, accurate model parameters are necessary in order to obtain the optimal operating condition. A first-order finite difference approximation was used for this simulation. The partial derivatives in z-direction are solved to ordinary differential equations (ODEs) by the method of lines (MOL). The result of numerical integration can be optimized by using MATLAB. The manipulated variable is flow rate of cooling water. The optimization study obtains that these set points of reactor's temperature can be calculated and controlled in a sufficiently performance. Moreover, this control can be developed in the future to reduce the operating cost and reactor size[8] or integrated with the EKF for estimating unmeasurable states and uncertain parameters or other mismatch cases for a higher robustness control and design.

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