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PREDICTIVE CONTROL OF BIODIESEL TRANSESTERIFICATION IN A BATCH REACTOR

CONTROL PREDICTIVO DE LA REACCIÓN DE TRANSESTERIFICACIÓN DE BIODIESEL EN UN REACTOR BATCH

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Abstract

Currently, the demand on fossil fuels continues increasing even though its use causes several damage to the environment. Biodiesel is a viable alternative to use of conventional diesel; however, biodiesel production is not always efficient and requires to satisfy quality standards. Automatic control improves the quality and efficiency on the production processes. Therefore, to improve productivity and ensure quality of the biodiesel production process in a batch reactor a predictive control strategy was implemented. The control strategy was based in the mathematical model of the reactor. This model describes the dynamics of the reaction and the energy during the production process. In the design of the control strategy, the boiling point restrictions of methanol and the operating range of the actuator were taken into account. The results shown that the products satisfied the requirement of ester content established in the norm EN 14214 and the reaction time was reduced by 42.86%. In addition, a better performance and lower heating flow consumption, regarding to conventional controller of type proportional integral, was shown by the predictive control system.

Keywords: biodiesel, transesterification, automatic control, model based predictive control.

Resumen

Actualmente, la demanda de combustibles derivados del petróleo sigue aumentando a pesar de que su uso causa graves daños al medio ambiente. El biodiésel es una alternativa viable para el uso del diésel convencional, sin embargo su producción no siempre es eficiente y requiere el cumplimiento de estándares de calidad. El control automático permite mejorar la calidad y la eficiencia de los procesos de producción. Por lo tanto, se implementó una estrategia de control predictivo al proceso de producción de biodiesel en un reactor discontinuo para mejorar la productividad y asegurar la calidad. La estrategia de control se basa en el modelo matemático del reactor. Este modelo describe la dinámica de la reacción y de la energía durante el proceso de producción. Durante el diseño de la estrategia de control se tomaron en cuenta las restricciones del punto de ebullición del metanol y el rango de operación del actuador. Los resultados mostraron que los productos cumplen con el requisito de contenido de éster establecido en la norma EN 14214 y que el tiempo de reacción se reduce en 42.86%. Además, el control predictivo mostró un mejor desempeño y un menor consumo de flujo de calentamiento, en comparación con controlador convencional tipo proporcional integral.

Palabras clave: biodiesel, transesterificación, control automático, control predictivo basado en modelo.

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1   Introduction

Nowadays, the world undergoes two great crises due to fossil fuel depletion and environmental destruction. The energetic crisis increases as world production of conventional oil begins to reach its limit and global demand of energy sources increase. From 2012 to 2013, oil global demand has increased 1.4%, while the world oil production has increased just by 0.6%. Because oil is a nonrenewable resource and there is a dependence on it as an energy source, it is the fossil energy source most likely to be consumed (Demirbas, 2008). According to the International Energy Study 2013 (Conti, 2013), global energy consumption will increase from 524 quadrillion BTU in 2010 to 820 quadrillion BTU in 2040; in addition, most of the energy used in the world still remains obtained from fossil fuels (almost 80% of the total predicted by 2040). Another alarming fact is that more than 90% of transport depends on fossil fuels. Additionally, excessive use of petroleum fuels has caused an environmental crisis. Dependence and excessive use of oil as an energy source has caused major environmental damage that is becoming irreversible. Gases produced by fossil-fuel combustion are the main cause of the "greenhouse effect". Climate change, thinning of the ozone layer and biodiversity loss are among the most serious consequences of excessive and disproportionate use of fossil fuels.

Along with the energy and environmental crisis, oil exhaustion has caused an economic crisis because its price increases as this energy source is being depleted. Thus, it is also causing an increase in the cost of its derivative products particularly fuels, such as diesel and gasoline.

Nevertheless, biodiesel is an alternative to diesel fuels (Katre *et al.*, 2012). The effects of its combustion do not cause major damage to environment because it reduces carbon dioxide emissions in 78.5% compared to diesel oil (Korotney, 2002). Biodiesel is a renewable resource (Meher *et al.*, 2006). Biodiesel advantage are biodegradability, higher flash point, reduction of exhaust emissions, miscibility with petrodiesel in all ratios, compatibility with existing fuel distribution infrastructure and inherent lubricity (Knothe and Steidley, 2011). However, biodiesel production is not always energetically and economically efficient. The reactor is the most important unit to be controlled in a biodiesel production plant because any variation in the standard operating conditions could impact the products (Ho *et al.*, 2010). On the other hand, the standard established for its use in diesel engines and

its commercialization have given rise to a greater attention to the development of control systems for its production process. Therefore, the automatic control techniques applied to the production of biodiesel have an important role in ensuring the quality of the product and optimizing its production process.

For this reason, Benavides and Diwekar (2012a) implemented a deterministic optimal control in a batch reactor that improved the biodiesel production by 1.47% and reduced the time production by 46%. Also, Benavides and Diwekar (2012b) applied to the same batch process a stochastic optimal control which improved the production in 1.67% with reduction of 43% in the production time. Likewise, Brásio *et al.* (2013) designed and implemented a nonlinear model predictive control for the production of biodiesel in a industrial scale semi-batch reactor. This automatic control system allowed to produce biofuel according the norm EN 14214 and to energetically and economically optimize the process.

Considering the foregoing, the design and implementation of a predictive control based on a model of batch reactor used in the biodiesel production process via transesterification of soybean oil with methanol is presented in this work. The main objective was to improve reactor productivity process by implementing a predictive control. The mathematical model for the reactor used in this work describes the dynamics of the reaction through mass balance (Noureddini and Zhu, 1997), and the dynamics of temperature from an energy balance (Kern and Shastri, 2015).

The predictive system controls the final concentration of biodiesel, so that it reaches a constant reference value, so it has a problem of regulation control. This reference value is determined from the simulation of the reaction at the optimum temperatures described in the literature (50 °C). The control variable is the heating water flow in the jacket.

In the literature it has been reported that a high reaction temperature increases the rate of biodiesel formation. But, the reactor temperature is limited by the boiling points of the reaction components (Noureddini and Zhu, 1997). Therefore, in the predictive control design, this variable of state is restricted. Moreover, the predictive control takes account the restriction over the range of reactor actuator. Finally, the performance of the predictive control designed and implemented in this work was compared with the performance of a conventional control in terms of the error and the consumption of

time and heating flow.

2 Mathematical model of biodiesel transesterification reactor
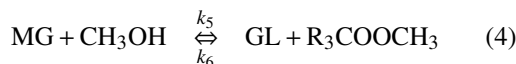
2.1 Modeling of the reaction

The most common biodiesel production method at small and medium scales is the vegetable oil transesterification reaction with alcohol (AL) in a batch reactor. Transesterification (also called alcoholysis) is the reaction of the triglycerides (TG) contained in an animal fat or vegetable oil with an alcohol to form esters (biodiesel) and glycerol (GL) (Ma and Hanna, 1999). Oils are mainly composed of triglycerides; generally, the 99% of refined soybean oil is TG (Pryde, 1980). In this study, the assumption is that oil consists of 100% of TG, and the terms oil and TG are indistinctly used, as well as ester or metyl ester and biodiesel. Also, during the transesterification reaction intermediates such as monoglycerides (MG) and diglycerides (DG) are formed (Kusdiana and Saka, 2001). In Eq (1), general transesterification reaction between methanol and TG from vegetable oil and methanol (CH$_3$OH) occurs. This shows that three methyl ester (ME) molecules or biodiesel (RCOOCH$_3$) and one molecule of GL are produced from the reaction of one molecule of TG with three molecules of methanol.

Overall reaction (Noureddini and Zhu, 1997):

$$TG + 3CH_3OH \overset{Catalyst}{\rightleftarrows} 3R_iCOOCH_3 + GL \quad (1)$$
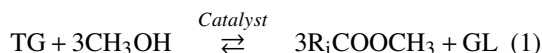
On the other hand, Eq (2)-(4) have three simultaneous reversible reactions that describe the step by step the overall reaction behavior, where k_{1-8} are rate constants. Transesterification is basically a sequential and simultaneous reaction. TG are first reduced to DG Eq (2). Then, DG are subsequently reduced to MG Eq (3). Finally, MG are reduced to fatty acid esters Eq (4) (Ma and Hanna, 1999).

Step by step reaction (Noureddini and Zhu, 1997):

$$TG + CH_3OH \underset{k_2}{\overset{k_1}{\Leftrightarrow}} DG + R_1COOCH_3 \quad (2)$$

$$DG + CH_3OH \underset{k_4}{\overset{k_3}{\Leftrightarrow}} MG + R_2COOCH_3 \quad (3)$$

$$MG + CH_3OH \underset{k_6}{\overset{k_5}{\Leftrightarrow}} GL + R_3COOCH_3 \quad (4)$$

From Eq (2)-(4), a system of differential equations describing the instantaneous speed of the reaction can be obtained. The general form of the governing set of differential equations characterizing the stepwise reactions involved in the TG transesterification are presented in Eq (5) - (10) (Noureddini and Zhu, 1997):

$$\frac{dC_{TG}}{dt} = -k_1C_{TG}C_{AL} + k_2C_{DG}C_{ME} \quad (5)$$

$$\frac{dC_{DG}}{dt} = k_1C_{TG}C_{AL} - k_2C_{DG}C_{ME} - k_3C_{DG}C_{AL} + k_4C_{MG}C_{ME} \quad (6)$$

$$\frac{dC_{MG}}{dt} = k_3C_{DG}C_{AL} - k_4C_{MG}C_{ME} - k_5C_{MG}C_{AL} + k_6C_{GL}C_{ME} \quad (7)$$

$$\frac{dC_{ME}}{dt} = k_1C_{TG}C_{AL} - k_2C_{DG}C_{ME} + k_3C_{DG}C_{AL} \quad (8)$$
$$- k_4C_{MG}C_{ME} + k_5C_{MG}C_{AL} - k_6C_{GL}C_{ME}$$

$$\frac{dC_{AL}}{dt} = -\frac{dC_{ME}}{dt} \quad (9)$$

$$\frac{dC_{GL}}{dt} = k_5C_{MG}C_{AL} - k_6C_{GL}C_{ME} \quad (10)$$

where C_i is the concentration of *i-th* reaction component (mol/L). Additionally, the reaction rate or reaction kinetics, k_i (1/s), is defined by the Arrhenius expression (11):

$$k_i(T) = a_i \exp\left(-\frac{E_i}{R_gT_R}\right), \text{ with } i = 1, 2, ..., 6 \quad (11)$$

where a_i is the pre-exponential factor which defines the frequency of collisions between molecules of the reactants (1/s), E_i is the activation energy of each component (J/mol), R_g is the universal constant for ideal gases (J/K mol) and T is the reactor temperature (K).

2.2 Modeling of the energy in the system

In this work a jacketed batch reactor which operates at atmospheric pressure and with constant volume is considered. The energy model used in this work was obtained from Kern and Shastri (2015) and it is presented in (12)-(13).

$$\frac{dT_R}{dt} = \frac{m_R}{V\rho C_p}\left(-V\frac{dC_{ME}}{dt}\Delta H_r + AU(T_j - T_R)\right) \tag{12}$$

$$\frac{dT_j}{dt} = \frac{1}{m_j}\left(f_h T_h + f_c T_c - (f_h + f_c)T_j - \frac{AU}{c_{pw}}(T_j - T_R)\right) \tag{13}$$

Where T_R is the reactor temperature, T_j is the jacket temperature, m_R is the mass in reactor, V is the reactor volume, c_p is the heat capacity of the reactor content, ρ is the density of the reactor content, ΔH_r heat of reaction, A is the jacket contact surface, U is the coefficient of heat transfer, m_j is the mass of water inside the reactor jacket , f_c and f_h are the mass flow of hot and cold water in the jacket, respectively, and c_{pw} the specific heat capacity of water.

In this way, the complete model of the reactor is given by the equations for the mass balances (5)-(10) and the energy balances (12)-(13).

3 Predictive control of biodiesel transesterification

Model based predictive control is an optimal control strategy. The optimization criterion is a cost function $V(k)$ which is related with the future behavior of the system. This behavior is predicted from a dynamic model or prediction model. The future time interval that is considered in prediction and optimization is called horizon prediction (H_p) and the prediction is performed starting from current time (k). The predicted behavior depends on the input applied to the system during the horizon prediction, $\hat{u}(k + i|k)$ for $i = 0, 1, \ldots, H_p - 1$ (Maciejowski, 2002). Thus on the optimization problem the decision variable is the input of the system. The basis of predictive control is to determine the signal input that produce the best predicted behavior to reach the desired state (set point). A reference signal is used in that case $r(k + i|k)$, which is the trajectory along which the system should reach to the set point signals at the end of H_p (Maciejowski, 2002).

The completed application of the optimal input signal generates a open loop control scheme. But through the sliding horizon technique, the control scheme becomes a close loop control system. The sliding horizon technique consists in applying the first element of the optimal input only for an instant. Then, the system status is sampled and the optimization problem is again solved. Thus, the horizon prediction slides over the time.

Also, model-based predictive control uses a time interval called as horizon control (H_u). This H_u regards the future time point when the control signal will be applied. The control horizon must not be greater than the prediction horizon H_u (i.e. $H_u \leq H_p$) because the main idea is that the output signal reaches the reference trajectory at the end of H_p.

3.1 Formulation of predictive control problem

The mathematical model of the system considered in this paper is a linear, discrete and time-invariant model. Moreover, this model is in state space form. Also, the assumption that the state vector is measurable and, therefore $x(k) = y(k)$), is made and there is no either perturbation or noise measuremente considered in the system. Therefore, the form of the prediction model used for predictive control in this work is presented in Eq (14).

$$x(k + 1) = Ax(k) + Bu(k) \tag{14}$$

where $x \in \mathbb{R}^n$ is the variables state vector, $u \in \mathbb{R}^p$ is the variables input vector (control signal), $A \in \mathbb{R}^{n \times n}$ is the state matrix and $B \in \mathbb{R}^{n \times p}$ is the input matrix. So, the prediction which is defined in Eq (15) is obtained by iteration of model Eq (14) (Maciejowski, 2002). Here $\Delta\hat{u}(k + i|k)$ is the changes in the input vector and it is defined as $\Delta\hat{u}(k + i|k) = \hat{u}(k + i|k) - \hat{u}(k + i - 1|k)$ for $i = 0, \ldots, H_u - 1$.

$$
\underbrace{\begin{bmatrix} \hat{x}(k+1|k) \\ \vdots \\ \hat{x}(k+H_u|k) \\ \hat{x}(k+H_u+1|k) \\ \vdots \\ \hat{x}(k+H_p|k) \end{bmatrix}}_{X(k)} = \underbrace{\begin{bmatrix} A \\ \vdots \\ A^{H_u} \\ A^{H_u+1} \\ \vdots \\ A^{H_p} \end{bmatrix}}_{\Psi} x(k) + \underbrace{\begin{bmatrix} B \\ \vdots \\ \sum_{i=0}^{H_u-1} A^i B \\ \sum_{i=0}^{H_u} A^i B \\ \vdots \\ \sum_{i=0}^{H_p-1} A^i B \end{bmatrix}}_{\Upsilon} u(k-1) + \ldots
$$

$$
\cdots + \underbrace{\begin{bmatrix} B & \cdots & 0 \\ AB+B & \cdots & 0 \\ \vdots & \ddots & \vdots \\ \sum_{i=0}^{H_u-1} A^i B & \cdots & B \\ \sum_{i=0}^{H_u} A^i B & \cdots & AB+B \\ \vdots & \vdots & \vdots \\ \sum_{i=0}^{H_p-1} A^i B & \cdots & \sum_{i=0}^{H_p-H_u} A^i B \end{bmatrix}}_{\Theta} \underbrace{\begin{bmatrix} \Delta\hat{u}(k|k) \\ \vdots \\ \Delta\hat{u}(k+H_u-1|k) \end{bmatrix}}_{\Delta\mathcal{U}(k)}
\tag{15}
$$

Predictive equation Eq (15) is used in a cost function which is the form of Eq (16) to perform the optimization implicated in the predictive control algorithm. This optimization problem is based in the minimization of the cost function.

$$
V(k) = \sum_{i=H_w}^{H_p} \| \hat{x}(k+i|k) - \hat{r}(k+i|k) \|^2_{Q(i)} + \sum_{i=0}^{H_u-1} \| \Delta\hat{u}(k+i|k) \|^2_{R(i)}
\tag{16}
$$

where $\hat{x}(k+i|k) - r(k+i|k)$ is a measurement of the error quantified during optimization. This error represent the difference between the predicted state and the reference signal. In addition $Q(i)$ and $R(i)$ are weighting matrices that penalize both the error and changes in the control signal. Also, H_w is the window parameter, which is used when it is not necessary to immediately start penalizing the error between x and r, because there may be some delay between applying an input and seeing any effect. In this case, the parameter H_w is established so that $H_w > 1$.

Optimization of cost function Eq (16) consists in error minimization which ensures that predictive control uses a minimum for the error $\hat{x}(k+i|k) - r(k+i|k)$ and changes in the control signal $\Delta\hat{u}(k+i|k)$.

A characteristic for the predictive control that makes it an attractive strategy for deal with the current complex processes is the possibility to establish constraints in the most important process variables.

There are three possible constraints in the applications of predictive control. First, two types of constraints deal with limitations in variables control $u(k)$, and the last type of constraint deals with limitations in variables output $y(k)$ or variables state $x(k)$. So constrains can be set in both, the movements and amplitude signal control, $\Delta u(k+i|k)$ and $u(k+i|k)$; as well as the system output $x(k+i|k)$. This constrains have the forms Eq (17)-(19) respectively.

$$
\Delta u_{min}(k+i|k) \leq \quad \Delta u(k+i|k) \quad \leq \Delta u_{max}(k+i|k) \tag{17}
$$
$$
u_{min}(k+i|k) \leq \quad u(k+i|k) \quad \leq u_{max}(k+i|k) \tag{18}
$$
$$
x_{min}(k+i|k) \leq \quad x(k+i|k) \quad \leq x_{max}(k+i|k) \tag{19}
$$

3.2 Solution of predictive control problem

The predictive control problem, which is an optimization problem for cost function Eq. (16), is defined in Eq (20).

$$
\min_{\Delta\hat{u}(k)} \sum_{i=H_w}^{H_p} \| \hat{x}(k+i|k) - \hat{r}(k+i|k) \|^2_{Q(i)} + \sum_{i=0}^{H_u-1} \| \Delta\hat{u}(k+i|k) \|^2_{R(i)} \tag{20}
$$

The cost function Eq (16) can be rewritten as it is shown bellow:

$$
V(k) = \| X(k) - \mathcal{T}(k) \|^2_Q + \| \Delta\mathcal{U}(kk) \|^2_{\mathcal{R}} \tag{21}
$$

with

$$\mathcal{T}(k) = \left[\hat{r}(k+H_w|k),\ldots,\hat{r}(k+H_p|k)\right]^T \quad (22)$$

$$Q(k) = diag\left[Q(H_w), Q(H_w+1),\ldots,Q(H_p)\right] \quad (23)$$

$$\mathcal{R}(k) = diag\left[R(0), R(1),\ldots,R(H_u-1)\right] \quad (24)$$

Likewise, the predictive equation Eq (15) can be rewritten as equation Eq. (25).

$$\mathcal{X}(k) = \Psi x(k) + \Upsilon u(k-1) + \Theta \Delta \mathcal{U}(k) \quad (25)$$

So replacing Eq (25) in Eq (21) and with some algebraic operations the cost function Eq (21) can be express as:

$$\begin{aligned} V(k) = & \mathcal{E}(k)^T Q \mathcal{E}(k) - 2\Delta \mathcal{U}(k)^T \Theta^T Q \mathcal{E}(k) \\ & + \Delta \mathcal{U}(k)^T [\Theta^T Q \Theta + \mathcal{R}]\Delta \mathcal{U}(k) \end{aligned}$$
$$(26)$$

where $\mathcal{E}(k) = \mathcal{T}(k) - \Psi x(k) - \Upsilon u(k-1)$. The new cost function Eq (26) has the following form:

$$V(k) = constant - \Delta \mathcal{U}(k)^T \mathcal{G} + \Delta \mathcal{U}(k)^T \mathcal{H} \Delta \mathcal{U}(k) \quad (27)$$

with

$$\mathcal{G} = 2\Theta^T Q \mathcal{E}(k) \quad (28)$$

$$\mathcal{H} = \Theta^T Q \Theta + \mathcal{R} \quad (29)$$

Therefore, the original control problem presented in Eq (20), which is expressed in term of cost function, becomes the optimization problem defined in Eq (30).

$$\min_{\Delta \hat{u}(k)} \Delta \mathcal{U}(k)^T \mathcal{H} \Delta \mathcal{U}(k) - \mathcal{G}^T \Delta \mathcal{U}(k) \quad (30)$$

Thus, the predictive control problem without constrains is solved when the solution for Eq (30) is found.

Now, to establish the constrained control problem is necessary to convert the original constrains Eq (17)-(19) to inequalities in function of the variable decision $\mathcal{U}(k)$. The process to transform this restriction is presented in the literature (Maciejowski, 2002; Wang, 2009). After the transformation, new restrictions has the form of Eq (31) (Maciejowski, 2002).

$$\Omega \Delta \mathcal{U} \le \omega \quad (31)$$

where Ω is a matrix and ω in a column vector. This way, the predictive control problem with constrains has the form of Eq (32), which is typical quadratic programming problem.

$$\min_{\Delta \hat{u}(k)} \Delta \mathcal{U}(k)^T \mathcal{H} \Delta \mathcal{U}(k) - \mathcal{G}^T \Delta \mathcal{U}(k) \quad (32)$$

subject to

$$\Omega \Delta \mathcal{U} \le \omega \quad (33)$$

4 Results and discussion

4.1 Reaction conditions and model parameters for simulation

The conditions for all simulations of the reaction that occurs in the reactor correspond to the transesterification of soybean oil with methanol in the presence of an alkaline catalyst. This conditions were obtained from literature and are presented in table 1 (Noureddini and Zhu, 1997). The parameters for the Arrhenius expression (11), that were used in every simulation of the reaction, are presented in table 2. This parameters were calculated from real experiments of the reaction at 50 °C (Noureddini and Zhu, 1997). Additionally, the parameters values from the energy model of the reactor (12)-(13) are shown in the table 1.

Table 1: Conditions for the transesterification reaction (Noureddini and Zhu, 1997)

Condition	Specification
Oil type	Soybean, refined
Molar relation (AL:TG)	6:1 mol/l
Alcohol type	Methanol
Reaction time	90 min
Catalyst	Sodium hydroxide
Catalyst concentration	0.20 wt% oil sodium hydroxide
Mix intensity	300 rpm

Table 2: Values for E_i and a_i in the Arrhenius equation (Noureddini and Zhu, 1997)

i	E_i (mol/L)	a_i (min)$^{-1}$
1	5.4999×10^4	3.8805×10^7
2	4.1555×10^4	5.7328×10^5
3	8.3094×10^4	5.6035×10^{12}
4	6.1250×10^4	9.7612×10^9
5	2.6865×10^4	5.3249×10^3
6	3.9991×10^4	2.0377×10^4

Table 3: Parameters of model energy (Fjerbaek et al., 2009; Patzek, 2009; Luus and Okongwu, 1999; Sorguven and Özilgen, 2010)

Parameter	Value	Units
ΔH_r	-18500	kJ/mol
ΔU	450	kJ/(min K)
ρ	860	kg/m^3
c_p	1277	kJ/(mol K)
c_{pw}	4.21	kJ/(mol K)
V	1	m^3
m_R	391.4	kg/mol
m_j	99.69	kg

4.2 Simulation of the transesterification reaction at constant temperature

Often, the transesterification reaction is carried out at constant temperature. In the literature, it has been reported that the optimum temperature for transesterification reaction at atmospheric pressure is between 50 °C and 60 °C (Leung *et al.*, 2010). However, there are reaction temperatures reported from -32 °C (Ma and Hanna, 1999). For this reason, a simulation of the reactor at different constant temperatures was performed to analise the effect of this variable on the conversion of triglicerydes into metil ester (biodiesel). The simulations were carried out from a temperature close to room temperature, that is, from 30 °C in increments of 10 °C to 60 °C. The effect of the temperature on the final state of reaction was analyzed, through the calculation of the mass percentage (%w/w). Assuming a perfect separation of glycerol, catalyst and alcohol, the methyl ester mass content was calculated from Eq (34) (Brásio *et al.*, 2013).

$$X_{ME} = \frac{m_{ME}}{m_{TG} + m_{DG} + m_{MG} + m_{ME}} \times 100\% \quad (34)$$

Figure 1 shows the evolution of mass content (formation) of methyl ester at different temperatures. As the temperature increases, the final mass percent of biodiesel is increased also. This is due to the high levels of energy in the reactant molecules during the reaction at higher temperatures, which favor the interaction between this molecules. Moreover, figure 1 show the effect of temperature on the reaction time.
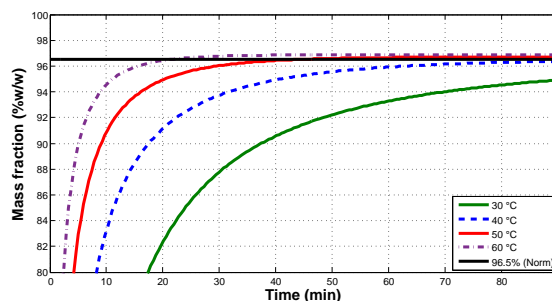

Fig. 1. Mass content of methyl ester at the different temperatures for biodiesel production.

The time reaction is reduced at the higher temperatures. This phenomena is due to the high energy levels on reactants and that the high temperature decrease the oil viscosities resulting in an increased reaction rate and a shortened reaction time (Benavides and Diwekar, 2012a). All of the above suggests that the temperature of the reaction should be as high as possible. However, this variable cannot be higher than the boiling point. This variable cannot be higher than the boiling point of methanol, which is the reactant with the lowest boiling point (64.7 °C). The final mass fraction of biodiesel is higher while the temperature is higher (see table 4). It can be seen that on the change from 30 °C to 40 °C the variation on X_{ME} was 1.0190%; while for the change from 50 °C to 60 °C, the X_{ME} variation was 0.1558%; i.e., the variation on X_{ME} was reduced more than 6 times. The limitation over the temperature reaction was considered in the design of predictive control system.

Table 4 shows the final mass percentages of biodiesel at different temperatures. These results show that the reaction products at 50 °C fulfill the norm specification EN 14214 for ester content (assuming a perfect separation of glycerol, catalyst and alcohol). At this temperature, the final mass percentage of metil ester was 96.71%, while the norm established a minimum mass content for fatty acid metil ester (without additives) of 96.5% (Brásio *et al.*, 2013). Therefore, the values of reaction products at 50 °C were used as set point signal for the predictive control.

4.3 Control design

A model based predictive control (MPC) strategy based on the linear model of biodiesel transesterification batch reactor was developed and implemented.

Table 4: Final mass fraction in percentage of biodiesel after the transesterification reaction at different temperatures

T(°C)	Percentage (%)
30	95.4356
40	96.4546
50	96.7173
60	96.9865

The objective of the control was to produce biodiesel that complies the 96.5% specification set in the norm EN 14214 for the ester content in the reaction products.

The control variables most used in chemical process are pressure, flow, level and temperature (e.g. temperatures of flow rates of cooling water in the coil or heating fluid in the jacket) (Benavides and Diwekar, 2012a). Since in this work a jacketed batch reactor is used which operates an atmospheric pressure and constant volume, the control variables are the heating and cooling flows in the jacket of the reactor (f_h and f_c, respectively) and the temperatures of flows in the input of the jacket (T_h and T_h, respectively). The heating flow was selected as the manipulated variable. This was done with the objective of evaluating the MPC performance with a conventional proportional integral (PI) controller, which allows to establish single control loops for only one variable.

Because the MPC control scheme uses a linear predictive model, the linearization of the nonlinear model [equations (5)-(10) y (12)-(13)] was carried out through the Taylor's series method. Then, in order to discretize the linear model obtained by the Taylor series method, the zero-order hold technique was used.

The simulation of the reaction at different constant temperatures shows that reaction products at 50 °C fulfill the norm specifications (96.5 %) for mass content of metil ester (see table 4). Thus, these values of products were used as nominal operation point. Likewise, the final mass content of metil ester was established as constant set point in the controls systems; therefore, there is a regulation-type control problem to consider.

The sampling period was establish as $T_s = 0.2$ min, which was calculated from the sampling theorem of Nyquist-Shannon. The predictive controller was designed with $H_P = H_u = 5$ (this is, 1 min). The weighting parameters were set as $Q(i) = 2.5 \times 10^5$ and $R(i) = 1.5$. All these parameters were tuned from trial and error, and simulations of the control system in a closed loop, with the objective to obtain a overshoot and steady stay negligible error in the control response (< 1%).

Because of the limitations on actuators of the reactor and physicochemical properties of the reactants, restrictions in the design of the MPC were established. Heating and cooling flows in the jacket vary in the range $f_{h,c} \in [0, 120]$ kg/min (Kern and Shastri, 2015). Therefore, in the MPC design the variations range of manipulable variable was restricted such that $0 \leq f_h \leq 120$ kg/min. The temperature of the reactor should not exceed the boiling point of methanol, which is the component with lower boiling point. Therefore, a restriction on reactor temperature (state variable) was set for a value a little lower of this point (64.7 °C), such that $T_R \leq 64$ °C.

The optimization problem (32) involved in the control problem, was solved using the quadratic programming with method of "interior-point-convex", in MATLAB® software.

The PI controller was tuned using the Ziegler-Nichols method. The tuning criteria for the PI were the same as for predictive control (overshoot and steady state error less than 1%). In this way, the calculated gains for PI were P=0.1613 and I=1.6131. To guarantee the restriction on f_h, a PI with saturation was implemented using as saturation limits $0 \leq f_h \leq 120$. However with PI it is not possible to impose constraints on the reactor temperature, but with the tuning obtained by the Ziegler-Nichols method this temperature does not exceed the boiling point limitation of methanol (see Fig. 5). Nevertheless, the capacity to establish restrictions on state variables (unlike conventional controllers), is one of the advantages of predictive control.

4.4 Control implementation

The performance of the MPC was evaluated against the performance of the PI and the performance of the reaction at a constant temperature of 50 °C. Figure 2 presents the evolution of the methyl ester mass fraction (in percentage) during the implementation of both control schemes and the open loop simulation of the reaction at constant temperature, as well as the 96.5% of the value required by EN14214 for this property. Both control systems reach the value required by the norm faster than the constant temperature reaction. The time to reach the required value was 24.8 minutes for MPC, 26.2 minutes for PI, and 43.4 minutes for the constant temperature reaction. This means that

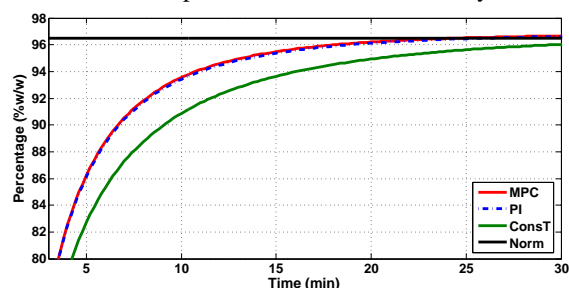MPC achieved a production time reduction by 42.86%

Fig. 2. Mass fraction in percentage obtained in simulation of: predictive control (MPC), proportional integral control (PI) and reaction at constant temperature (ConsT); and the value for norm EN 14214.
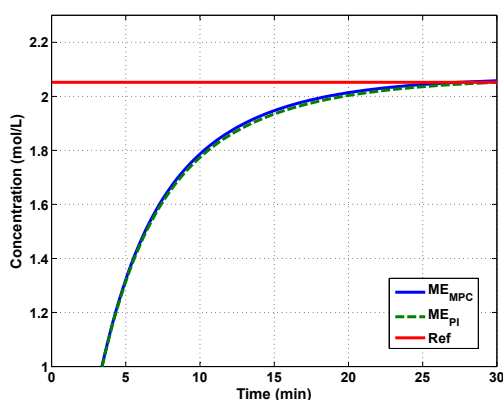

Fig. 3. Concentration of methyl ester (output signal) during control implementation and signal of reference for both controllers. ME_{MPC}, output signal for predictive control. ME_{PI}, output signal for proportional integral control. Ref, signal of reference for both controllers.

compared to the constant temperature reaction, while the PI control system improved this time in 39.63%. That is, the predictive control decreased 3.23 % more the time to reach the norm than the integral proportional controller, with respect to the reaction at constant temperature. A direct comparison between both controllers shows that the MPC reduces the time of the norm by 5.34 % in relation with the PI.
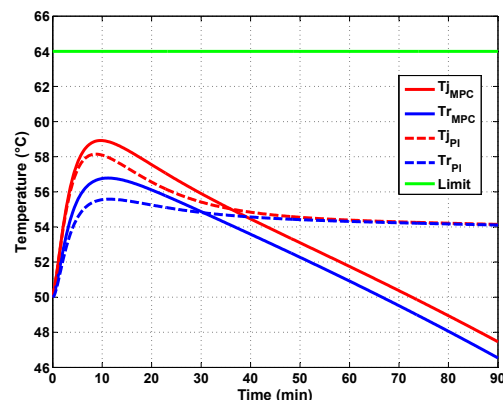

Fig. 4. Reactor and jacket temperatures. Tj_{MPC} and Tr_{MPC}, temperatures in the jacket and reactor with MPC implementation, respectively; Tj_{PI} and Tr_{PI}, temperatures in jacket and reactor with PI implementation, respectively; Limit, constraint for boiling point of methanol.

Figure 3 shows the output signals from the control systems and the reference signal. Both signals follow a similar trajectory to reach the reference value. However, the predictive control reaches the reference in a shorter time than the conventional control. Settling time (2%) was lower for the predictive control (19.4 minutes), in relation to proportional integral control (23.2 minutes).

Table 5 presents the "Integral Absolute Error" (IAE) obtained by the control systems during the settling time. The predictive control model had an IAE index of 75.62 mol/l, while PI had an IAE index of 77.25 mol/l. Thus, better performance was obtained by the predictive control as compared to the traditional controller.

Figure 4 shows the evolution of reactor and jacket temperatures during the implementation of control systems. The reactor temperature does not exceed the limit of 64 °C. The maximum value reached for reactor temperature by the MPC controller was 58.9 °C, while the PI reached 56.7 °C. In both cases the reactor temperature was below the limit value.

Table 5: Implementation result of control systems

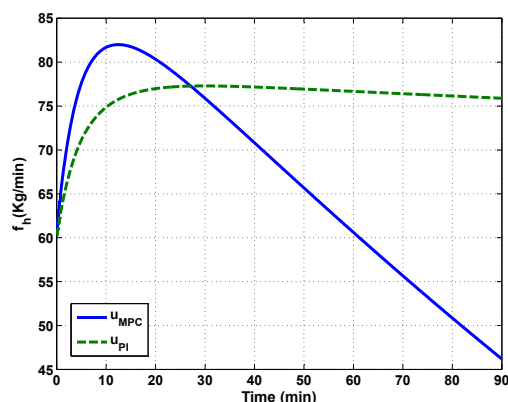| Strategy	Time of norm (min)	Setting time (min)	IAE (mol/L)	Consumption of hot fluid (L)
MPC	24.8	19.4	75.62	6009.5
PI	26.2	23.2	77.25	6846.7

Fig. 5. Control signals of two different control systems during the operation of transesterification reactor.

In figure 5 the control signals of both control systems are presented. In both cases, the control signal did not reach the limits for the heating flow ($f_h \in [0, 120]$). It can be observed that the predictive control signal is higher in relation to integral proportional control, during the first 27 min. During this time, it reaches a maximum value of 82 kg/min. After this time, it decreases with rate of 0.495 kg/min in each minute, until reaching the value of 46.18 kg / min. For the other hand, the PI control signal increases until the value of 77.29 kg/min during first 30 minutes. Then, it slowly declines on average rate of 0.0335 kg/min per minute, until reaching the value of 75.89 kg/min. Taking into account the total simulation time (90 min), the consumption of the heating flow by the MPC was 6009.5 liters of water. For its part,the proportional integral control used 6846.7 liters. This represents a greater consumption by the PI, which is 12.23 % higher than the utility water consumption using the MPC.

Conclusion

In this paper, a model based predictive control system for biodiesel transesterification in a batch reactor was implemented. The reaction was carried out from soy oil and methanol. The complex dynamics present in the biodiesel production reactor require a nonlinear model of the system. The nonlinear model of the system was formulated by the mass and energy balances to the reactor. This model was linearized and used as a predictive model in the predictive control design. Also, the limitations present in the reactor, which were established due to the boiling point of the methanol and the range of actuator action, were taken into account during the design of the control.

The performance of the predictive control system was evaluated against a proportional integral controller and the reaction operation at a constant temperature. The predictive control system showed an improvement in the production process in comparison to the conventional controller, as it allowed producing biodiesel according to specification of ester content, established in the norm EN 14214 and with a reduction of 42.86% in the production time, while the PI based controlled has led to a reduction of 39.63%. Additionally, the proportional integral controller signal showed a higher energy consumption. This controller shown a higher consumption of the heating flow by 12.23% compared to the MPC.

In this way, the predictive control proved to improve the productivity of the biodiesel production process by reducing production time and satisfying the ester content specification of EN 14214. In addition, MPC controller performs this task in a better way and with a better performance compared to conventional controller, because the implementation result analysis showed that the MPC achieves a lower IAE index and consumption of hot fluid (1.63 $mol \cdot L^{-1}$ and 837.2 L, respectively).

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