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OPTIMAL TEMPERATURE CONTROL FOR ETHANOL FERMENTATION IN A BATCH REACTOR

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การเพิ่มขึ้นของราคาน้ำมันที่ต้องนำเข้าจากต่างประเทศ ทำให้ต้องหาแหล่งพลังงานทางเลือกหนึ่งในทางเลือกที่เป็นไปได้คือการใช้เอทานอล ซึ่งเอทานอลจะสามารถแข่งขันกับน้ำมันแก๊สโซลีนโดยปราศจากการแทรกแซงราคาได้ ถ้าค่าใช้จ่ายในการผลิตเอทานอลต่ำกว่าราคาน้ำมันแก๊สโซลีน ดังนั้นงานวิจัยนี้จึงเสนอการประยุกต์ใช้การควบคุมแบบออพติมัลเพื่อหาโพรไฟล์ที่เหมาะสมที่สุดของอุณหภูมิในเครื่องปฏิกรณ์แบบกะสำหรับการหมักเอทานอล การควบคุมอุณหภูมิแบบออพติมัลถูกนำมาใช้เพื่อให้ได้ปริมาณของเอทานอลที่มากที่สุดในตอนสิ้นสุดกระบวนการหมัก ซึ่งปัญหาการควบคุมอุณหภูมิแบบออพติมัลหาคำตอบได้โดยใช้วิธีการแบบลำดับขั้น ผลการศึกษาพบว่าการควบคุมอุณหภูมิแบบออพติมัลให้ค่าของปริมาณเอทานอลในตอนสิ้นสุดกระบวนการมากที่สุดเมื่อเทียบกับกระบวนการอื่น จากนั้นได้ศึกษาผลกระทบของช่วงเวลาที่ใช้เพื่อปรับปรุงสมรรถนะการควบคุม นอกจากนี้ได้ใช้การวิเคราะห์ทางเศรษฐศาสตร์เบื้องต้นของค่าใช้จ่ายในการผลิตเอทานอลเพื่อเปรียบเทียบผลที่ได้ระหว่างระบบที่ใช้การควบคุมอุณหภูมิแบบออพติมัลกับระบบที่ใช้อุณหภูมิคงที่ที่ 31.02 องศาเซลเซียส ผลการวิเคราะห์พบว่าค่าใช้จ่ายในการผลิตต่อหน่วยของระบบที่ใช้การควบคุมอุณหภูมิแบบออพติมัลค่อนข้างต่ำกว่าระบบที่ใช้อุณหภูมิคงที่ และกำไรต่อหน่วยของระบบที่ใช้การควบคุมอุณหภูมิแบบออพติมัลสูงกว่าระบบที่ใช้อุณหภูมิคงที่ จากผลการศึกษาแสดงให้เห็นว่าการควบคุมอุณหภูมิแบบออพติมัลสามารถช่วยปรับปรุงกระบวนการหมักเอทานอลให้ดำเนินการได้อย่างมีประสิทธิภาพ

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NIWAT CHANASUTHIPRAPA: OPTIMAL TEMPERATURE CONTROL FOR ETHANOL FERMENTATION IN A BATCH REACTOR.

THESIS ADVISOR: ASST.PROF.MUENDUEN PHISALAPHONG, Ph.D.,

THESIS CO-ADVISOR: AMORNCHAI ARPORNWICHANOP, D.Eng. 82 pp.

Increases in imported crude oil prices have led to seeking alternative resources. One of the possible solutions is to use the ethanol as an alternative. Ethanol can compete with gasoline, without any intervention, if its total production cost is lower than the gasoline's price. Therefore, this research presented the application of an optimal control for the temperature profile of a batch reactor in ethanol fermentation. The optimal temperature control strategy was applied to obtain the maximum amount of the desired ethanol product at the end of the operation. The solution of the optimal temperature control problem was computed using a sequential approach. It was found that the optimal temperature control provides the best value of final ethanol concentration among other processes. Later on, the effects of time interval were investigated in order to improve the control performance. In addition, preliminary economic analysis on the operating cost was used to compare the results between the system with the optimal temperature control and the isothermal process (31.02°C). The results showed that the unit operating costs of the system with optimal temperature control was relatively lower than that of the isothermal process and the unit profit of the system with the optimal temperature control was to a certain extent higher than that of the isothermal process. These results demonstrated that the optimal temperature control technique assist the ethanol fermentation process operates effectively.

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NOMENCLATURES

C_P	ethanol concentration (g/L)
C_{P0}	initial ethanol concentration (g/L)
C_S	substrate concentration (g/L)
C_{S0}	initial substrate concentration (g/L)
C_X	cell concentration (g/L)
C_{X0}	initial cell concentration (g/L)
J	performance index
K_{CM}	maintenance constant (h^{-1})
K_d	specific cell death rate (h^{-1})
K_S	saturation growth constant (g/L)
K_{SP}	saturation production constant (g/L)
K_{SS}	substrate growth inhibition term (g/L)
K_{SSP}	substrate production inhibition term (g/L)
P_m	ethanol inhibition term for growth (g/L)
P'_m	ethanol inhibition term for production (g/L)
$Y'_{P/S}$	yield coefficient for product on substrate used for produce
$Y'_{X/S}$	yield coefficient for cells on substrate used for cell formation
x	the vector of state variables
u	the vector of control variables
μ	specific growth rate (h^{-1})
μ_m	maximum specific growth rate (h^{-1})
ν	specific production rate (h^{-1})
ν_m	maximum specific production rate (h^{-1})

CHAPTER I

INTRODUCTION

1.1 Background

The increasing of fuel cost is a critical economic problem in Thailand. Ethanol has re-emerged as an alternative to or extender for petroleum based liquid fuels. To reduce the country's dependence on costly imported fuel and to assist in creating a new domestic fuel industry, the Thai government initiates use ethanol as additive for gasoline to form a mixture which is commonly known as gasohol. The advantages of using ethanol as an alternative fuel are to increase combustion efficiency and to reduce the petroleum-derived fuels demand.

To effectively operate the ethanol fermentation process, the kinetic characteristics of cell are necessary for controlling the process. Temperature is one of the most important factors because temperature has strong effects on the kinetic parameters of ethanol fermentation. Therefore optimal control technique is used to determine a temperature profile for operation which yields the maximum amount of desired products at the end of operational time.

The optimal control (also known as dynamic optimization problem) is optimization problems based on dynamic models of the system. The solutions of optimal control problems have been a subject of researches for many years (Srinivasan et al., 2003). There are several different computational techniques available for solving the optimal control problems. The indirect or variational approaches based on the first order necessary conditions for optimality obtained from Pontryagin's Maximum Principle (Pontryagin et al., 1962). However, it has been found that these approaches result to a two-point boundary value problem which is difficult to solve.

Thus the direct approaches which transform the original optimal control problem into a finite dimensional nonlinear programming problem (NLP) and solve it directly have been proposed. Depending on the degree of discretization, the direct approaches can be classified into two groups. In the sequential approaches, only the control variables are discretized (Edgar and Himmelblau, 1988) whereas in the simultaneous approaches, the control and state variables are discretized (Biegler, 1984).

This study aims to develop optimal control strategy for controlling temperature of a batch reactor in ethanol fermentation and use preliminary economic analysis to compare the results between the system with optimal temperature control and isothermal process.

1.2 Objective

1) Develop optimal control strategy for controlling temperature of a batch reactor in ethanol fermentation.

2) Preliminary economic analysis to compare the results between the system with optimal temperature control and isothermal process.

1.3 Benefit of Research

The outcome of this research provided the optimal temperature strategy for high ethanol production.

1.4 Scope of Research

1) Previous mathematical model in a batch reactor described ethanol fermentation by the flocculating yeast, *Saccharomyces cerevisiae* M30 and using cane molasses as the substrate (Phisalaphong et al., 2006) is studied by simulations.

2) A mathematical model for optimal control technique is developed to determine a temperature policy for the batch reactor.

3) Sequential approach is used to solve optimal control problem.

4) Preliminary economic analysis on the operating cost is used to compare the results between the system with optimal temperature control and isothermal process.

5) MATLAB program is used to simulate process and solve optimal control problem. An economic analysis on the operating cost of process is performed with HYSYS process simulation software.

This thesis is divided into six chapters:

Chapter I is an introduction of this research. This chapter consists of background, objective, benefit of research and scope of research.

Chapter II presents the literature reviews with temperature effect on ethanol fermentation, optimal control and the optimal control of ethanol fermentation.

Chapter III describes the theoretical background of the ethanol production processes and the optimal control.

Chapter IV presents the application of optimal temperature control for ethanol fermentation in a batch reactor.

Chapter V presents the preliminary economic analysis on the operating cost.

Chapter VI presents the conclusions of this research. Future work and the recommendations are also stated

CHAPTER II

LITERATURE REVIEWS

2.1 Temperature Effect on Ethanol Fermentation

In ethanol fermentation processes, the temperature is one of the most important factors of the fermentation. Because temperature has strong effects on the kinetic parameters of ethanol fermentation. The influences of temperature on ethanol fermentation have been a subject of researches for many years. Torija et al. (2003) studied the influence of fermentation temperature (from 15 to 35 ^{0}C) on a mixed strain population. They used Mitochondrial DNA analysis to differentiate *Saccharomyces cerevisiae* strains and determine the frequency of each strain during the alcoholic fermentation. The results showed that some strains performed better at high temperatures and others at low temperatures. Viable cells decreased at high temperatures, especially at 35 ^{0}C. They claimed that alcohol yield was higher at low temperatures and secondary metabolites to alcoholic fermentation increased as the temperature increased.

In addition, Sánchez et al. (2004) studied the influence of temperature between 10 and 40 ^{0}C on the fermentation of *d-xylose* with *Pachysolen tannophilus* ATTC 32691 to produce ethanol and xylitol. They claimed that the highest values for overall ethanol yield and the specific ethanol-production rate were obtained for fermentations carried out at 30 ^{0}C, which was also quite close to the optimum temperature for the formation of biomass. Maximum overall xylitol yield occurred at 15 ^{0}C.

Besides, Phisalaphong et al. (2006) developed a mathematical model to describe the effects of temperature on the kinetic parameters of ethanol fermentation by using the flocculating yeast, *Saccharomyces cerevisiae* M30, and cane molasses as a substrate. They established Arrhenius relationships between operating temperature and the maximum specific growth rate, specific production rate, specific death rate. Polynomial equations were established for the effects of temperature on the other kinetic parameters. The results showed that a high temperature led to a decreased in the ethanol and cell yields but an increased in the inhibition effect of ethanol and sugar on cell growth and ethanol production.

Moreover, Rivera et al. (2006) used optimization techniques to estimate the kinetic model parameters of batch fermentation process for ethanol production using *Saccharomyces cerevisiae*. Batch experimental observations at five temperatures (28, 31, 34, 37 and 40 ^{O}C) were used to formulate the parameter estimation problem. The potential of Quasi-Newton (QN) and Real-Coded Genetic Algorithm (RGA) to solve the estimation problem was considered to find out the optimal solution. Subsequently, the optimized parameters were characterized by correlation functions assuming temperature dependence. They claimed that the kinetic models optimized by QN and RGA described satisfactorily the batch fermentation process as demonstrated by the experimental results.

Furthermore, Cazetta et al. (2007) analyzed ethanol production from sugar cane molasses under different culture conditions using *Z. mobilis* in batch fermentation. They claimed that the best conditions for ethanol production were 200 g/L of total reducing sugars, temperature of 30 ^{0}C, and static culture for 48 h, achieving 55.8 g /L of ethanol.

Finally, Table 2.1 displays the overview of study in temperature effect on ethanol fermentation.

Table 2.1 The overview of study in temperature effect on ethanol fermentation

Authors	Details
Torija et al. (2003)	Studied the influence of fermentation temperature on a mixed strain population of ethanol fermentation.
Sánchez et al. (2004)	Studied the influence of temperature on fermentation of d-xylose with *Pachysolen tannophilus* to produce ethanol and xylitol.
Cazetta et al. (2007)	Analyzed ethanol production from sugar cane molasses under different culture conditions using *Z. mobilis* in batch fermentation.
Phisalaphong et al. (2006)	Developed a mathematical model to describe the effects of temperature on the kinetic parameters of ethanol fermentation by using the *Saccharomyces cerevisiae*, and cane molasses as a substrate.
Rivera et al. (2006)	Used optimization techniques to estimate the kinetic model parameters of batch fermentation process for ethanol production which assuming temperature dependence.

2.2 Optimal Control

Optimal control involves determining a control profile for a dynamic system that optimizes a given performance index. There were many researches which involved using optimal control strategy for several processes. Yoon et al. (1989) studied the optimal temperature policy for a multi-stage immobilized enzyme reactor system and enzyme deactivation during continuous reactor operation was considered for optimization. They used optimal control strategy to

find optimal temperature profile for maximizing productivity. They found that as the number of stages increased, productivity also increased and the high productivity in the multi-stage reactor system was also obtainable in a single-stage reactor system if multi-compartment temperature control could be provided along the reactor column as in the multi-stage reactor system.

Moreover, Cacik et al. (2001) presented the application of an optimal control procedure to reduce the fermentation time necessary to produce a desired amount of xanthan gum. They used this procedure to compute the temperature operating policy for the culture based on the fermentation initial conditions and the desired product concentration at the final time. The results showed that the optimal fermentation time to produce 15 g of gum/L was 16.3 % shorter than the necessary time when the usual constant temperature of 28 °C was used and 12% shorter than the necessary time when the two-temperature strategy of other authors (Shu and Yang, 1991) was used.

In addition, Aziz et al. (2002) developed optimal operation policies in batch reactors using dynamic optimization technique. They formulated two different types of optimization problems, namely, maximum conversion and minimum time problems and solved to obtain optimal operation policies in terms of reactor temperature or coolant flow rate. A path constraint on the reactor temperature was imposed for better reactor operation and an endpoint constraint on undesired waste production (by-product) was imposed to minimize environmental impact.

Furthermore, Ming Xie et al. (2002) investigated the optimization of temperature and feed control strategies for glycerol production by fed-batch culture of osmophilic yeast *Candida krusei* to maximize the final yield whilst to control the residual glucose at a low concentration. They divided the entire fermentation process into multi-subintervals for convenient control performance and easy numerical solution. Both piecewise-constant temperature (PCT) and

discrete-pulse feed (DPF) control strategies were optimized by the complex method of Box based on previous macro-kinetic model and verified experimentally in a 600 ml airlift loop reactor. It was found that, by model-based optimization of only DPF control strategies, the final glycerol yield were significantly improved compared with those by previous empirical strategies.

Besides, Arpornwichanop et al. (2005) developed an approach, based on an on-line dynamic optimization strategy, to modify optimal temperature set point profile for batch reactors. They formulated two different optimization problems concerning: maximization of product concentration and minimization of batch time and solved using a sequential optimization approach. To update current states from their delayed measurement and to estimate immeasurable state variables an Extended Kalman Filter (EKF) was incorporated into the proposed approach. A nonlinear model-based controller: generic model control algorithm (GMC) was applied to drive the temperature of the batch reactor following the desired profile. The proposed approach was applied for a batch reactor with complex exothermic reaction scheme. The results showed that with the proposed strategy, large improvement in batch reactor performance, in term of the amount of a desired product and batch operation time, could be achieved compared to the method where the optimal temperature set point was pre-determined.

Furthermore, Kawohl et al. (2007) addressed the application and comparison of model based estimation, optimization, and control methods for fed-batch bioprocesses. The estimation quality of two constrained optimization based state estimation algorithms, namely the Bayesian maximum a posteriori based Constrained Extended Kalman-Filter (CEKF) and the Moving-Horizon-State-Estimation (MHE) was compared to the classical unconstrained Extended Kalman-Filter (EKF). They claimed that the MHE shows higher potential for state estimation in small systems, for high order systems the adjustment of the filter parameters and the numerical optimizations were more intricate. Table 2.2 shows the overview of study in optimal control.

Table 2.2 The overview of study in optimal control

Authors	Details
Yoon et al. (1989)	Studied the optimal temperature policy for a multi-stage immobilized enzyme reactor system and enzyme deactivation during continuous reactor operation was considered for optimization.
Ming Xie et al. (2002)	Investigated the optimization of temperature and feed control strategies for glycerol production by fed-batch culture of osmophilic yeast *Candida krusei*.
Aziz et al. (2002)	Developed optimal operation policies in batch reactors using dynamic optimization technique and solved to obtain optimal temperature profile.
Arpornwichanop et al. (2005)	Developed an approach, based on an on-line dynamic optimization strategy, to modify optimal temperature set point profile of batch reactor system.
Cacik et al. (2001)	Presented the application of an optimal control procedure to reduce the fermentation time necessary to produce a desired amount of xanthan gum.
Kawohl et al. (2007)	Addressed the application and comparison of model based estimation, optimization, and control methods of fed-batch bioprocesses for the production of antibiotics.

2.3 Optimal Control for Ethanol Fermentation

Many attempts have been made to apply optimal control strategies for ethanol fermentation. Teng Wu et al. (1993) implemented and applied an on-line optimal control strategy for ethanol production. They used optimal control with a quadratic performance index to carry out process and the dilution rate as the manipulated variable. The results showed that the better utilization of substrate was obtained by using the optimal control. Toro et al. (1997) used optimal control technique to find optimal temperature profile in beer fermentation. They solved optimal control problem by Genetic Algorithm (GA) and they claimed that GA could be used to provide an optimum temperature profile for industrial beer fermentation.

Moreover, Acosta et al. (1999) applied a non-linear optimization, based on a stochastic multi-start search algorithm to maximize the production rates of ethanol, glycerol and carbohydrates. This optimization was applied to two alternative (non-linear) model representations of the same system, namely the Michaelis–Menten and the generalized mass action forms. They found a complete agreement between the results obtained using both representations.

Besides, Valentinotti et al. (2003) analyzed the maximization of biomass productivity in the fed-batch fermentation of *Saccharomyces cerevisiae*. They used a novel adaptive control methodology based on the internal model principle to maintain the desired ethanol setpoint. The experimental results demonstrated the effectiveness of the proposed control methodology. Trelea et al. (2004) demonstrated the possibility of obtaining various desired final aroma profiles and reducing the total process time using dynamic optimization of three control variables: temperature, top pressure and initial yeast concentration in the fermentation tank. The optimization was based on a sequential quadratic

programming algorithm, on a dynamic model of the alcoholic fermentation and on an aroma production model.

In addition, Gee et al. (2004) applied optimal control theory to the process of batch beer fermentation. The performance functional considered was a weighted sum of maximum ethanol production and minimum time. They determined model parameters from isothermal batch fermentations. The fermentor cooling duty was the single available control. Temperature state variable constraints as well as control variable constraints were considered. The optimal control law was shown to be bang-bang control with the existence of a singular arc corresponding to isothermal operation at the maximum temperature constraint.

Besides, Xiong et al. (2005) proposed strategy to overcome the problems of unknown disturbances and model-plant mismatches in fed-batch process optimal control through online re-optimization. They applied neural network-based discrete-time models to model fed-batch processes from process operation data. Due to the existence of unknown disturbances and model-plant mismatches, the off-line calculated “optimal” feeding policy for the remaining batch period might no longer be optimal and should be re-optimized. Thus a modified iterative dynamic programming algorithm based on discrete-time nonlinear models was developed to solve the on-line re-optimization problem.

Furthermore, Shomchoam (2006) implemented an on-line optimal control with neural network estimator to control the feed rate in a fed-batch reactor for production of ethanol. He coped with unknown disturbances and model-plant mismatches by developed on-line optimal control. Artificial neural network was used to estimate unmeasured state variables which were employed as feedback information of the system. He formulated optimal control problem and solved by a sequential method in which the control profile was parameterized by using a piecewise constant function. The simulation results have shown that the on-line optimal control with neural network estimator gave a better control performance in

terms of the amount of the desired ethanol product, compared with the off-line optimal control. The overview of study in optimal control for ethanol fermentation was shown in Table 2.3.

Table 2.3 The overview of study in optimal control for ethanol fermentation

Authors	Details
Teng Wu et al. (1993)	Implemented and applied an on-line optimal control strategy to control dilution rate for ethanol production.
Xiong et al. (2005)	Proposed strategy to overcome the problems of unknown disturbances and model-plant mismatches to control feed rate for ethanol production through online re-optimization with neural network.
Shomchoam (2006)	Implemented an on-line optimal control with neural network estimator to control the feed rate in a fed-batch reactor for production of ethanol.
Toro et al. (1997)	Used optimal control technique to find optimal temperature profile in beer fermentation.
Trelea et al. (2004)	Demonstrated the possibility of obtaining various final aroma profiles and reducing total process time using dynamic optimization of temperature, pressure and initial yeast concentration in fermentation tank.
Acosta et al. (1999)	Applied a non-linear optimization, based on a stochastic multi-start search algorithm to control feed rate for maximize the production rates of ethanol, glycerol and carbohydrates.
Valentinotti et al. (2003)	Analyzed the maximization of biomass productivity in the fed-batch reactor for ethanol fermentation by control the substrate feed rate.
Gee et al. (2004)	Applied optimal control theory to control cooling water flowrate in the isothermal batch reactor for beer fermentation.

CHAPTER III

THEORETICAL BACKGROUND

In this chapter, the theoretical background of the ethanol production processes, the process economics, the mathematical modeling and the optimal control are described.

3.1 Ethanol Production Processes

Ethanol, also known as ethyl alcohol or grain alcohol, is a flammable, colorless, mildly toxic chemical compound with a distinctive perfume-like odor. Its molecular formula is C_2H_6O, variously represented as EtOH, C_2H_5OH or as its empirical formula C_2H_6O (Streitweiser et al., 1976).

3.1.1 Categories of Ethanol Production

Ethanol is produced both as a petrochemical, through the hydration of ethylene, and biologically, by fermenting sugars with yeast or bacteria.

- **Ethylene hydration**

Ethanol for use as industrial feedstock could also make from petrochemical feed stocks, typically by the acid-catalyzed hydration of ethylene, represented by the chemical equation

$$C_2H_4 + H_2O \rightarrow CH_3CH_2OH \qquad (3.1)$$

The catalyst is most commonly phosphoric acid, adsorbed onto a porous support such as diatomaceous earth or charcoal; this catalyst was first used for large-scale ethanol production by the Shell Oil Company in 1947. Solid catalysts,

mostly various metal oxides, have also been mentioned in the chemical literature (Lodgsdon, 1994).

In an older process, first practiced on the industrial scale in 1930 by Union Carbide (Lodgsdon, 1994), but now almost entirely obsolete, ethene was hydrated indirectly by reacting it with concentrated sulfuric acid to product ethyl sulfate, which was then hydrolyzed to yield ethanol and regenerate the sulfuric acid:

$$C_2H_4 + H_2SO_4 \rightarrow CH_3CH_2SO_4H$$
$$CH_3CH_2SO_4H + H_2O \rightarrow CH_3CH_2OH + H_2SO_4 \qquad (3.2)$$

- **Fermentation**

Generally, ethanol for use in alcoholic beverages and fuel is produced by fermentation: when certain species of yeast (most importantly, *Saccharomyces cerevisiae*) metabolize sugar in the absence of oxygen, they produce ethanol and carbon dioxide. The overall chemical reaction conducted by the yeast may be represented by the chemical equation

$$C_6H_{12}O_6 \rightarrow 2\ CH_3CH_2OH + 2\ CO_2 \qquad (3.3)$$

The process of culturing yeast under conditions to produce alcohol is referred to as brewing. Brewing can only produce relatively dilute concentrations of ethanol in water; concentrated ethanol solutions are toxic to yeast. The most ethanol-tolerant strains of yeast can survive in up to about 25% ethanol by volume (Clines, 2007).

During the fermentation process, it is important to prevent oxygen getting to the ethanol, since otherwise the ethanol would be oxidized to acetic acid (vinegar). Also, in the presence of oxygen, the yeast would undergo aerobic respiration to produce just carbon dioxide and water, without producing ethanol.

Ethanol is made from a variety of agricultural products such as grain, molasses, fruit, whey and sulfite waste liquor. Generally, most of the agricultural products mentioned above command higher prices as foods, and others, e.g., potatoes, are uneconomical because of their low ethanol yield and high transportation cost. The energy crisis of the early seventies may have generated renewed interest in ethanol fermentation, but its use still depends on the availability and cost of the carbohydrate relative to the availability and cost of ethylene. Sugar and grain prices, like oil prices, have risen dramatically since 1973.

Fermentation processes from any material that contains sugar can derive ethanol. The many and varied raw materials used in the manufacture of ethanol via fermentation are conveniently classified under three types of agricultural raw materials: sugar, starches, and cellulose materials. Sugars (from sugar cane, sugar beets, molasses, and fruits) can be converted to ethanol directly. Starches (from grains, potatoes, root crops) must first be hydrolyzed to fermentable sugars by the action of enzymes from malt or molds. Cellulose from wood, agricultural residues, waste sulfite liquor from pulp and paper mills) must likewise be converted to sugars, generally by the action of mineral acids. Once simple sugars are formed, enzymes from yeast can readily ferment them to ethanol. The data of raw materials as shown in Table 3.1 (Keim, 1983).

Table 3.1 Fermentation fuel ethanol - potential raw materials

Sugar-containing	Starch-containing	Cellulosics	Other
Sucrose & invert	Cereal grains	Wood	Jerusalem artichoke
Molasses	Corn	Sawdust	Banana
Sugar beet	Grain sorghum	waste paper	Alcohol-containing
Sugar cane	Wheat	Forest residues	Wine surplus
Sweet sorghum	Barley	Agricultural residues	Brewers' yeast
Fruit, juice	Milling Products	Municipal solid waste	Brewery waste
Lactose	Wheat flour		
Whey	Wheat millfeeds		
Glucose	Corn horminy		
Sulphite waste	Starchy roots		
	Mandioca		
	Potatoes		

3.1.2 Industrial Fermentation Processes

Whatever the raw material or the specifications of the alcohol product to be made, all commercial fermentation ethanol processes are composed of several steps:

(1) Preparation of the raw material.
(2) Hydrolysis, in the case of starches and cellulosics.
(3) Fermentation.
(4) Recovery and concentration of alcohol.
(5) Recovery of by-products.

There are many different ways of performing each of these steps and scores of variations within each alternative.

(1) Preparation of the raw material

All raw materials must be prepared prior to fermentation. Sugar-containing products require the least preparation and the steps involved are relatively simple, such as dilution, filtration, and adjustment of pH or temperature. Of the sugar materials, molasses may require the greatest amount of pretreatment; because of the large amount of non-fermentables it contains (Table 3.2).

Table 3.2 Typical composition of cane molasses (percent by weight at 75% ds)

	Usual range (%)	Average
Fermentable sugars	48 - 56	52
Other organic material	9 - 12	10.5
Inorganic ash	10 - 15	12.5
Dry substance		75
Water		25
Total		100

(Source: Composition, Properties and Uses of Molasses and Related Products, United Molasses Trading Company Limited, London)

In the group of starchy raw materials, grains and roots must all be pretreated by cleaning and size reduction at least, and often by some degree of starch purification as well. When wheat flour is used, the pretreatment usually involves the removal of protein in the valuable form of vital gluten, leaving a relatively purified starch for the alcohol process.

The situation is different for the cellulose-containing raw materials, where the physical structure makes it extremely difficult to release the cellulose and pretreated it for easy accessibility by the hydrolyzing agent. Preparation methods suggested for these materials include fine grinding, roll milling, separation by building up internal steam pressure with heat and then releasing it explosively, or by chemical methods similar to those used in pulp mills.

(2) Hydrolysis, in the case of starches and cellulosics

After the preliminary preparation, starch or cellulosic materials must be hydrolyzed to form fermentable sugars, and this may be accomplished with acid, enzymes or a combination of both. The hydrolysis may be carried out completely before the fermentation is started, partially beforehand and completed in the fermenters, or entirely during fermentation, a procedure called Simultaneous Saccharification and Fermentation, or SSF.

Starch is much easier to hydrolyze than cellulose and the technology and equipment for doing it commercially have been developed over a long time by starch converters and equipment suppliers. The starch industry hydrolyses large amounts of commercially pure starch, using acid, acid enzyme, or dual-enzyme processes to make low, regular, and high DE (dextrose equivalent) syrups, crystallized dextrose (D-glucose monohydrate or anhydrous D-glucose) or highly converted and purified glucose syrups used as substrates for isomerization to high-fructose corn syrups (HFCS or Iso-Syrup). In the US the wet-milling plants are using these techniques to produce fermentables for alcohol, and the whole grain plants are also adopting these methods.

A number of specific processes and equipment units have been proposed, or are being used to hydrolyze starch in alcohol plants. However, in all of them the starch must first be cooked in water, where a slurry of starch is heated, the granules absorb water and the slurry viscosity increases until a critical temperature has been reached, after which the viscosity drops dramatically as the starch molecules become solubilized. The temperature range of highest viscosity varies with the source of the starch, but, in general, is lower for root starches and higher for the grains. Cereal starches often contain a small portion of granules that require temperatures well in excess of 100°C to be fully solubilized.

When solutions of cooked starch are cooled, longer molecules tend to aggregate (retrograde), forming many intermolecular and intramolecular associations that are not reactive to commercial saccharifying enzymes. Thus, it is extremely important that during the cooking phase the starch not only be gelatinized but also that the degree of polymerization (DP) be reduced enough to prevent retrogradation on cooling. This is accomplished by hydrolyzing to at least 10-12 DE with acid or α-amylase, either of which randomly cuts starch molecules into shorter lengths. This step is usually referred to as liquefaction.

After liquefaction by either acid or a-amylase, the temperature may safely be reduced for further hydrolysis with glucoamylase (amyloglucosidase), which operates best at 60-65°C and pH 4.0-4.5. Its action is a stepwise removal of glucose molecules from the non-reducing end of carbohydrate chains, and this process is known in the industry as saccharification. This hydrolysis starts rapidly, but then slows to the point where with normal enzyme concentrations as much as 72 hours treatment time is required to achieve maximum saccharification.

(3) Fermentation

After the raw material has been prepared and hydrolysed, it is ready for fermentation, where enzymes provided by yeast break down simple sugars primarily into ethanol and carbon dioxide, with the evolution of heat. Processes for accomplishing this have been developed over the centuries, and although they were satisfactory for the types and quantities of alcohol previously produced, they fall well short of ideal for the scale of operation required for fuel alcohol. Here, methods are needed to minimize both investment and operating cost per unit of alcohol produced, by maximizing fermentation rates and alcohol yields.

To accomplish this, great attention must be paid to detail, since improper design and/or operation may easily reduce yields by 20% or more below stoichiometry. The main causes for losses are

- Failure to disperse fully the carbohydrate.
- Incomplete saccharification.
- Formation of unfermentable sugars.
- Diversion of carbohydrate to yeast growth and cell maintenance.
- Diversion of carbohydrate to products other than ethanol.

In a typical fermentation, a selected yeast is added to the sugar-containing solution in a vessel provided with heat exchangers to remove the heat given off during fermentation. As the reaction proceeds, ethanol and carbon dioxide are formed, the CO_2 passing out of the vessel while the alcohol concentration increases. However, other events occur at the same time. One is the biological activity of the yeast itself, where some of it dies, while more grows. In this process, the yeast transforms nitrogen (either added as a nutrient or already present in the substrate, e.g. the protein in grain) into protein, while consuming as much as 6% of the sugars, which are then unavailable for making alcohol.

Furthermore, yeast fermentations produce other organic compounds besides ethanol and carbon dioxide, the most important of which is glycerol. This major loss of yield becomes even worse if the pH is allowed to rise or if bisulphite ion is present. In addition, significant amounts of organic acids, acetaldehyde and fusel oils are formed, the last two usually being left in for fuel alcohol but removed for beverage and pure industrial grades. Another potential major loss of alcohol yield occurs when bacteria are able to invade and establish yet more reactions. For all these reasons, optimum commercial fermentation designs must maintain yeast vitality while suppressing excess growth, the growth of bacteria and the formation of extraneous products.

Industrially used yeasts are strains of bakers' or brewers' yeast (*Saccharomyces cerevisiae*) selected to provide the best possible combination of characteristics for the process and equipment being used, with greatest importance being attached to tolerance to high concentrations of sugars and alcohol. These

yeasts normally operate best at pH ~ 4.5 and 28-30°C, with efficiency dropping off rapidly at higher temperatures. Since the fermentation is exothermic, the substrate must be cooled, and in large plants this often becomes a major operation and cost factor.

(4) Recovery and concentration of alcohol

Ethanol is recovered from the fermented substrate by fractional distillation. The number, dimensions and types of columns employed vary greatly according to the designer and the specifications of the alcohol to be produced. Nevertheless, in all cases the first step is to strip the alcohol from the supply stream, leaving an absolute minimum in the bottoms (stillage). This stripping (or 'beer') column usually contains a few rectifying plates which concentrate the alcohol in the overhead to some 50-70%.

In traditional plants, the distillate is condensed and passed through a series of redistillations and recondensations to reach the desired product quality. In such systems, consumption of energy in the form of steam is very large. This large steam consumption led to the largely irrelevant question being raised of whether alcohol production is energy inefficient, and increased the cost estimates of producing it with expensive steam.

The concentration of the alcohol is then finally upgraded to be 95-96 % by weight, by a distillation method. The alcohol with 95-96% concentration is normally called "hydrous alcohol", which can fuel only specially designed vehicles such as flex fuel cars. However, ethanol, with a purpose to be blended with gasoline, for uses in general vehicles, must be anhydrous ethanol (99.5% alcohol concentration). Thus, the residual remaining water in hydrous alcohol must be removed by a dehydration process. Currently; a molecular sieve technique is a common technique to separate the water out from the ethanol to produce anhydrous alcohol.

(5) Recovery of by-products

In general, the ethanol production of sugar base crops yields three main by-products: stillage, fusel oil and carbon dioxide. Stillage is a residual beer remaining in the distillation waste, after the alcohol has completely been removed from the distillation columns. During the distillation process, there are two types of distillates obtained from the distillation columns: fusel oil, and alcohol. Fusel oil is a higher order of one type of alcohol with more than two carbons in its molecular structure, and it is formed during the fermentation, in conjunction with the ordinary alcohol with two carbons in its molecular structure.

Ethanol production from starch based crops gives one more by-product, i.e., Distiller's Dried Grain (DDG). DDG is the unfermented materials which are recovered and dried together as Distiller's Dried Grain. On a commercial basis, this product contains at least 27% protein plus appreciable amounts of oil and fat, hence it is a valuable feed for animals, especially dairy cattle.

CO_2 is generated during the anaerobic sugar fermentation. The CO_2 produced from the fermentation is almost equally to the amount of the ethanol produced in the fermentation process, by weight.

In some cases, the carbon dioxide is collected and sold for use in freezing food, carbonating beverages, charging fire extinguishers, making dry ice and various other uses. However, in the US very large amounts of carbon dioxide are derived as a by-product of ammonia manufacture, and its value is very low near these sources, which actually vent most of their production. The value in other locations is at least the cost of loading and transporting from the ammonia plants. The situation is being changed by decreased ammonia production and increased interest in the use of large amounts of carbon dioxide in flooding old oil fields for tertiary recovery of petroleum.

The steps of the ethanol production as mentioned above are summarized and shown in Figure 3.1.

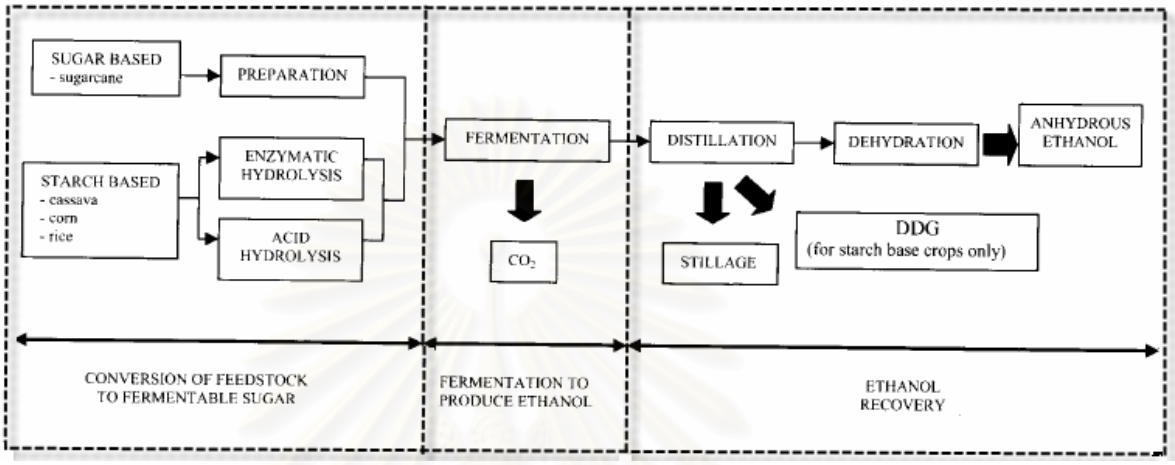

Figure 3.1 anhydrous ethanol production processes (Yoosin et al., 2007)

3.1.3 Process Economics

The processing costs of the ethanol can be categorized into four major groups: capital costs, feedstocks costs, operating & maintenance costs, and by-product gains.

(1) Capital costs

Capital investment represents the first costs of all necessary equipment in production and their installations. Expenses for piping, instrumentation, insulation, foundations and site preparation are included in the capital costs. In addition, these costs also include land, buildings and waste treatment facilities. Normally, the capital investment for a new plant includes two main items:

1. The direct costs include the costs of all machines and equipment, as well as their installation cost, land, main plant building, laboratories, offices and warehouses, instrumentation and piping works.
2. The indirect costs include engineering consulting costs and their contingency allowances.

(2) Feedstocks costs

Feedstock prices can vary by location, seasons, local conditions of the supply-demand, and transportation. These market price variables can affect a decision in selecting a feedstock type for ethanol production. The prices of the feedstocks as shown in Table 3.3. The feedstocks cost is the most significant expense that affects the cost of manufacture (Seider et al., 2004).

Table 3.3 The maximum, minimum and average of the feedstock costs in baht per ton and baht liter of ethanol from 2002 to 2005 (Yoosin et al., 2007)

Feedstock	Maximum		Minimum		Average	
	Baht /$ton_{feedstock}$	Baht /l_{EtOH}	Baht /$ton_{feedstock}$	Baht /l_{EtOH}	Baht /$ton_{feedstock}$	Baht /l_{EtOH}
Cassava	1,370	8.56	920	5.75	1,096	6.85
Corn	4,800	12.80	4,472	11.92	4,668	12.45
Rice	5,698	15.19	4,106	10.95	4,728	12.61
Sugarcane	577	8.24	440	6.29	494	7.06
Molasses	4,800	20	3,000	12.5	3,800	15.83

(3) Operating & maintenance costs

The operating and maintenance costs are: labor, energy, electricity, ingredients (e.g. enzymes, yeasts, etc.), repairs and maintenance, waste disposal, taxes, insurance cost, and administrative expense.

Table 3.4 Operating cost items and ranges (Petrides, 2000)

COST ITEM	Type Of Cost	Range of values (% of total)
A. Raw Materials	Direct	10-80
B. Labor	Direct	20-50
C. Consumables	Direct	1-50
D. Lab/QC/QA	Direct	2-50
E. Waste Disposal	Direct	1-20
F. Utilities	Direct	1-30
G. Equipment-Dependent	Indirect	10-70
H. Miscellaneous	Indirect	0-20

Table 3.4 displays the various types of operating costs, their direct or indirect nature, and ranges for their values relative to the total operating cost. Sometimes cost items are categorized as either fixed or variable. Fixed costs are those that are incurred regardless of volume of product output. The clearest case of a fixed cost is depreciation, which is part of the equipment-dependent cost. The clearest case of a variable cost would be the cost of raw materials. Most other costs have a fixed and a variable component.

(4) By-product gains

The fermentation process of the ethanol production also yields several byproducts, including carbon dioxide, fusel oil, yeasts and stillage. The by-products of the ethanol production can generate additional incomes. In other words, they assist to reduce the ethanol production cost, significantly, provided that they are economically recovered, effectively. The byproducts are dependent

on the types of feedstocks and processing methods used in the ethanol production. Logically, the type of co-products depends on the type of employed feedstock as shown in Table 3.5.

Table3.5 Current and potential added-value co-products that can be obtained during fuel ethanol production (Cardona, 2007).

Co-product	Process	Stage where co-product is formed	Application
Yeast	Ethanol from sugar cane	Centrifugation of culture broth after fermentation	Cattle feed supplement
Bagasse	Ethanol from sugar cane	Crushing of sugar cane	Feedstock for production of animal feed, enzymes,aminoacids, organic acids,etc.
Fructose	Ethanol from sugar cane	Selective fermentation coupled with pervaporation	Sweetener for food industry
CCDS	Corn wetmilling process	Evaporation of thin stillage (liquid fraction obtained)	Food for non-ruminants (poultry and swine)
DDGS	Corn dry milling process	Combination of evaporated thin stillage and solids obtained after centrifugation	High value feed for ruminants containing 27–35% protein
Xylitol	Biomass-toethanol process	Xylose solutions obtained during pretreatment of lignocellulosic biomass can be converted into xylitol by chemical or biotechnological	Anticariogenic sweetener

CCDS, corn condensed distiller's solubles.

DDGS, dried distiller's grains with solubles.

3.1.4 Batch Fermentation

Batch fermentation is a system that is fermented by microorganism within close fermentor by limiting nutrient. The nutrient is feeding only once time at the beginning of the fermentation process. The nutrient and product are removed at the ending of the fermentation process. The microbial growth in the batch fermentation can be divided in five phase; a lag phase, a growth phase, a production phase, a stationary phase and a declining phase. During the lag phase, microorganisms spend time for suitable adaptation to substrate. Figure 3.2 shows the principle time course of cell mass, substrate and product concentration for different types of fermentation

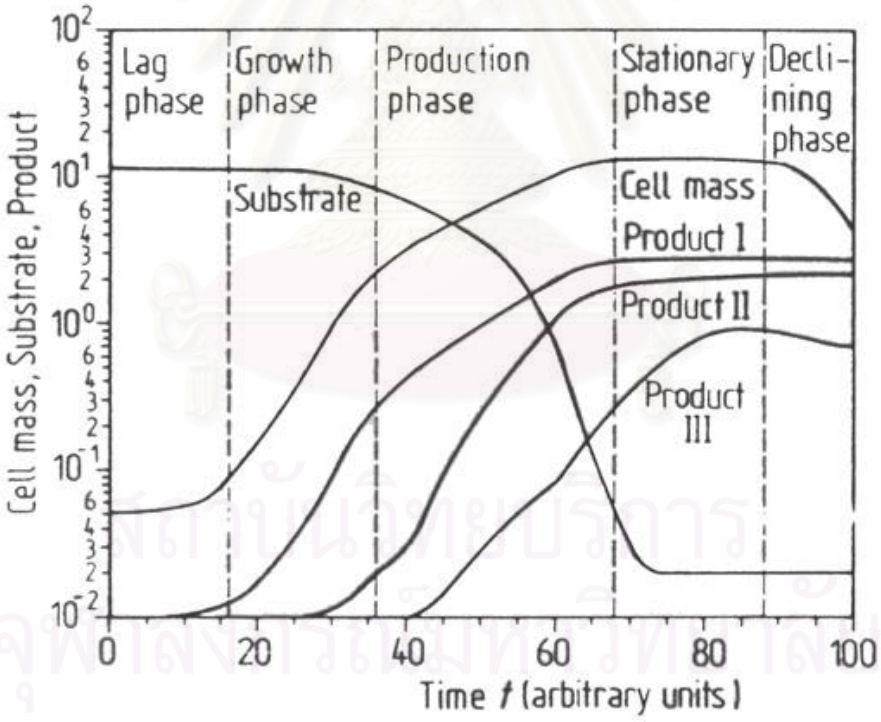

Figure 3.2 Principal time course of cell mass, substrate and product concentration for different types of fermentation
(Source: Kehm et al., 2001)

3.1.5 Mathematical Modeling

Mathematical modeling for cell activities is an important part in design and fermentation process development. It can be specified by depending on complexity contemplation. Considering of the mechanism in cells, chemical and biochemical reactions, included transport phenomena and energy transfer in cells and also phase and component in fermentation, specification of mathematic model in fermentation must concern nearly real conditions. However, ideal situation for creating reality model is unreachable so the assumptions are made.

Generally, batch fermentation can be set and written in mathematic equations by growth, substrate utilization and production as in the following equations.

Cell mass balance in batch fermentation

rate of biomass concentration change	=	rate of biomass concentration change caused by exponential growth

$$\frac{dC_x}{dt} = \mu(C_x, C_s, C_p, T)C_x \qquad (3.4)$$

Substrate utilization in batch fermentation, integrated by using coefficient yield from cell growth

rate of substrate concentration change	= −	rate by which the substrate is consumed by micro-organism	−	rate by which the substrate is utilized by production

$$\frac{dC_s}{dt} = -\frac{1}{Y_{x/s}}\mu(C_x, C_s, C_p, T)C_x - m_s C_x - \sum_j \frac{r_{Pj}}{Y_{Pj/s}} C_x \qquad (3.5)$$

Substrate utilization in batch fermentation, integrated by using coefficient yield from cell growth

rate of product concentration change	=	rate of product synthesis

$$\frac{dC_p}{dt} = \frac{1}{Y_{x/p}}\mu(C_x, C_s, C_p, T)C_x \qquad (3.6)$$

where

C_X	cell concentration
C_S	substrate concentration
C_P	product concentration
μ	specific growth rate
m_s	maintenance constant
T	temperature
$Y_{P/S}$	yield coefficient for product on substrate
$Y_{X/S}$	yield coefficient for cells on substrate

A well known model to describe biomass growth is the Monod model (Monod, 1942). The Monod model can be written as:

$$r_x = \mu_{max} \frac{C_s C_x}{K_s + C_s} \tag{3.7}$$

$$r_s = -\frac{r_x}{Y_{xs}} \tag{3.8}$$

where

μ_{max} maximal specific growth rate

K_S Monod-constant

Y_{XS} yield of biomass production on substrate

The Monod model is probably the most often used equation to describe biomass growth. Some alternative equations have also been proposed. Table 3.6 shows alternative growth kinetics for a single substrate.

Table 3.6 Growth kinetics for a single substrate

Name	Year	Normalized Kinetics
BLACKMAN	1905	$\mu_{max} \frac{C_s C_x}{K_s + C_s}$
TEISSIER	1942	$\mu_{max} \frac{C_s C_x}{K_s + C_s}$
CONTOIS	1959	$\mu_{max} \frac{C_s C_x}{K_s + C_s}$
MASON and MILLS	1976	$\mu_{max} \frac{C_s C_x}{K_s + C_s}$

(Source: Kehm et al., 2001)

3.2 Optimal Control Theory

The objective of optimal control theory is to " *determine the control signals that will cause a process to satisfy the physical constraints and at the same time minimize (or maximize) some performance criterion."* (Kirk, 1970)

3.2.1 Problem Formulation

In batch process operations, the process variables undergo significant changes during the duration of batch. There is no steady state and thus no constant set point around which the process can be regulated. Hence, the major objective in batch operations is not to keep the system at some optimal constant set point, but rather to optimize an objective function that expresses the system performance (Palanki et al., 1993). Batch process optimization problems involve both dynamic and static constraints and fall under the class of optimal control problem.

Optimal control, also known as a dynamic optimization problem, involves determining a control profile for a dynamic system that optimizes a given performance index. The dynamic system is usually represented by sets of differential and algebraic equations (DAEs) derived from dynamic mass and energy balances, and physical and thermodynamic relations.

A general optimal control problem can be stated as follows:

Find $u(t)$ over $t \in [t_0 , t_f]$ maximizing or minimizing

$$J = \theta[x(t_f)] + \int_{t_0}^{t_f} \varphi[x(t), u(t), t]dt \tag{3.9}$$

Subject to

$$\frac{dx}{dt} = f\left[x(t), u(t), t\right] \tag{3.10}$$

$$x(t_0) = x_0 \tag{3.11}$$

$$h\left[x(t), u(t), t\right] = 0 \tag{3.12}$$

$$g\left[x(t), u(t), t\right] \leq 0 \tag{3.13}$$

$$x^L \leq x(t) \leq x^U \tag{3.14}$$

$$u^L \leq u(t) \leq u^U \tag{3.15}$$

where J is the performance index or desired objective function, x and u are the vector of state and control variables, respectively, Eq. (3.10) is the system of ordinary differential equations, Eq. (3.11) is the initial condition for Eq. (3.10), Eqs. (3.12) and (3.13) are the equality and inequality algebraic constraints, respectively, and Eqs. (3.14) and (3.15) are the upper and lower bounds on the state and control variables, respectively.

There are several different computational techniques available for solving the optimal control problems. The indirect approaches based on the first order necessary conditions for optimality obtained from Pontryagin's Maximum Principle (Pontryagin et al., 1962). These approaches are also known as variational approaches. However, it has been found that these approaches result to a two-point boundary value problem which is difficult to solve. Thus, the direct approaches which transform the original optimal control problem into a finitedimensional nonlinear programming problem and solve it directly are proposed. Depending on the degree of discretization, the direct approaches can be classified into two general strategies. In the simultaneous approaches, the control and state variables are discretized (full discretization) whereas only the control variables are discretized (partial discretization) in the sequential approaches.

3.2.2 Sequential Approaches

This approach is also referred to as Control Vector Parameterization (Edgar and Himmelblau, 1988). In this approach, the input is parameterized using a finite set of decision variables. Thus, the optimization is carried out in input variables only. Typically, a piecewise constant approximation over equally spaced time intervals is made for the inputs. Given the initial conditions, the process equations are solved with a differential algebraic equation solver. This produces the value of the objective function, which the optimization routine then iteratively uses to find the optimal parameters in the control parameterization. The sequential approach is of the feasible path type, that is, in every iteration, all process equations are feasible during the calculation of the objective value. This leads to a robust solution procedure if a first feasible solution is given first.

The general algorithm of the sequential approaches is as follows:

Problem:

$$\min_{u(t)} \Phi\left[x(t), u(t), t\right]$$

Subject to

$$\frac{dx}{dt} = f\left[x(t), u(t), t\right]$$

$$x(0) = x_0 \tag{3.16}$$

$$h\left[x(t), u(t), t\right] = 0$$

$$g\left[x(t), u(t), t\right] \le 0$$

$$x^L \le x(t) \le x^U$$

$$u^L \le u(t) \le u^U$$

Step 1: Discretize the process inputs using any standard collocation method (e.g. orthogonal collocation).

$$u_K(t) = \prod_{i=1}^{k} u_i \psi_i(t) \quad \text{where} \quad \psi_i(t) = \prod_{k=1,i}^{k} \frac{(t - t_k)}{(t_i - t_k)}, u_K(t_i) = u_i \qquad (3.17)$$

Step 2: Substitute the parameterized inputs into the process dynamic model

$$\begin{aligned} &\frac{dx}{dt} = f\left[x(t), u_K(t), t\right] \\ &i = 1,...,K \\ &\text{with} \quad x(0) = x_0 \end{aligned} \qquad (3.18)$$

Step 3: Substitute the modified process dynamic model given by Eq. (3.17) into the problem given by Eq. (3.16). The updated problem statement according to sequential approaches is given by Eq. (3.19).

$$\underset{u(t)}{\text{Min}}\, \Phi\left[x(t), u(t), t\right]$$

subject to

$$\frac{dx}{dt} = f\left[x(t), u_K(t), t\right] \quad \text{when } i = 1,...,K$$

$$u_K(t) = \prod_{i=1}^{k} u_i \psi_i(t) \quad \text{where} \quad \psi_i(t) = \prod_{k=1,i}^{k} \frac{(t - t_k)}{(t_i - t_k)}, u_K(t_i) = u_i$$

$$x(0) = x_0 \qquad (3.19)$$

$$h\left[x(t), u(t), t\right] = 0$$

$$g[x(t), u(t), t] \leq 0$$

$$x^L \leq x(t) \leq x^U$$

$$u^L \leq u(t) \leq u^U$$

Step 4: Choose t_i using orthogonal collocation method and evaluate u as a function of time by using Eq. (3.17).

Step 5: Choose initial guess for decision variables and solve the dynamic process model given by Eq. (3.18) in Step 2 for the input obtained in step 4 using any ODE solver (e.g. Runge-Kutta or Newton-Raphson Methods).

Step 6: Evaluate the objective function given in Eq. (3.19) using state and control profiles obtained in step 5 and update the values of decision variables using any standard optimization routine such as steepest descent or Quasi- Newton methods. Repeat steps 4 through 6 until convergence.

The main advantage of the sequential approaches is that only the control profiles are discretized and considered as the decision variables. The optimization formulated by this approach is a small scale nonlinear programming problem. However, the limitation of these approaches is a difficulty to handle a constraint on state variables. This is because the state variables are not directly included in the nonlinear programming problem. The quality of the solution is strongly dependent on the parameterization of the control profile. The solution converges quickly only if a feasible solution is given as a starting guess. However to find this feasible solution is a non-trivial problem.

3.2.3 Simultaneous Approaches

Although sequential approaches guarantee an optimal solution by following a feasible path, they can be prohibitively expensive because they tend to converge slowly and require solution of differential equation at each iteration. The simultaneous approach avoids this calculation by simultaneously converging to the optimum while solving the differential equations. In the simultaneous approaches, both state and control variable profiles are discretized by approximating functions and treated as decision variables in the optimization problem. The process dynamic models and the optimization problems are solved at the same time. Orthogonal collocation is applied to the system of differential equations to convert them into a set of algebraic equations. Then, an optimization strategy was applied at each iteration that did not require satisfaction of equality constraints at each iteration (Biegler, 1984).

The general algorithm for the simultaneous approaches is as follows:

Problem:

$$\underset{x(t),u(t)}{\text{Min}}\ \Phi\left[x(t),u(t),t\right]$$

Subject to

$$\frac{dx}{dt} = f\left[x(t),u(t),t\right]$$

$$x(0) = x_0 \tag{3.20}$$

$$h\left[x(t),u(t),t\right] = 0$$

$$g\left[x(t),u(t),t\right] \le 0$$

$$x^L \le x(t) \le x^U$$

$$u^L \le u(t) \le u^U$$

Step 1: Discretize the process states and inputs using any standard collocation method (e.g. orthogonal collocation).

$$x_{K+1}(t) = \sum_{i=0}^{K} x_i \phi_i(t) \quad \textit{where} \quad \phi_i(t) = \prod_{k=0,i}^{K} \frac{(t - t_k)}{(t_i - t_k)}, x_{K+1}(t_i) = x_i \tag{3.21}$$

$$u_K(t) = \prod_{i=1}^{k} u_i \psi_i(t) \quad \text{where} \quad \psi_i(t) = \prod_{k=1,i}^{k} \frac{(t - t_k)}{(t_i - t_k)}, u_K(t_i) = u_i$$

Step 2: Substitute the discrete states and inputs into process dynamic model and obtain the algebraic expression for residuals.

$$R(t_i) = \sum_{j=0}^{K} x_j \phi_j(t_i) - f(x_i, u_i, t_i) = 0$$

$$i = 1,\ldots,K \tag{3.22}$$

$$\text{with} \quad x(0) = x_0$$

Step 3: Substitute the discretized dynamic model into the original optimal control problem.

$$\underset{x(t),u(t)}{\text{Min}} \; \Phi[x(t), u(t), t]$$

subject to

$$R(t_i) = \sum_{j=0}^{K} x_j \phi_j(t_i) - f(x_i, u_i, t_i) = 0 \quad \text{when } i = 1,\ldots,K$$

$$x(0) = x_0 \tag{3.23}$$

$$h\left[x(t), u(t), t\right] = 0$$

$$g\left[x(t), u(t), t\right] \le 0$$

$$x^L \le x(t) \le x^U$$

$$u^L \le u(t) \le u^U$$

Step 4: Choose t_i by using orthogonal collocation method.

Step 5: Solve problem given in Step 3 at the t_i chosen in Step 4 using any non-linear programming problem solver such as Successive Quadratic Programming (SQP).

The main advantage of the simultaneous approaches is that approximate optimal solutions can be achieved starting from a very poor initial guess. On the other hand, the main disadvantage of the approaches is that the resultant static optimization problem has a large number of unknown variables, and may be plagued with many local minima. Thus, computing the global minimum may be difficult, and as a consequence direct approaches tend to give inaccurate solutions.

3.2.4 Variational Approaches

These approaches are based on the solution of the first order necessary conditions for optimality that are obtained from Pontryagin's Maximum Principle (Pontryagin, 1962). The Pontryagin's Maximum Principle based approaches convert the original scalar objective function involving states and inputs into a Hamiltonian involving states, inputs and adjoint states. These procedures lead to a

two-point boundary value problem (TPBVP) that can be solved with different approaches, including single shooting, multiple shooting, invariant embedding or some discretization methods such as collocation on finite elements or finite differences. The limitation of these approaches is the complexity in the solution of differential-algebraic equations.

CHAPTER IV

APPLICATION OF OPTIMAL TEMPERATURE CONTROL FOR ETHANOL FERMENTATION IN A BATCH REACTOR

In this chapter, the mathematical model of ethanol fermentation process in a batch reactor is presented. In addition, the application of optimal temperature control strategy for ethanol fermentation in a batch reactor is studied.

4.1 Mathematical Model of Ethanol Fermentation in a Batch Reactor

Mathematical modeling of fermentation processes can be classified into two main categories namely, structured and unstructured models. In unstructured models, the biomass is regarded as a chemical compound in a solution with an average formula. In structured models, biomass is regarded as a number of biochemical compounds, thus, taking into consideration the change in internal composition of the organism.

For decades, the expression of cell kinetic has been developed in many ways. The best model is close to realistic condition; however, it has much complexity in the calculation. Among the various modes of the fermentation such as continuous, batch and fed-batch modes, the batch mode is used to implement for this study.

In the current study, the mathematical model developed by Phisalaphong et al. (2006) for describing the effects of temperature on the kinetic parameters of ethanol fermentation by using the flocculating yeast, *Saccharomyces cerevisiae* M30, and cane molasses as the substrate. This mathematical model that could describe the dynamic process of ethanol fermentation. The model modified from the Monod kinetics responding to changes in the environmental conditions. The proposed kinetics was modified in both substrate and product terms and combined with death rate and cell maintenance. Since ethanol fermentation was an anaerobic process, thus the dissolve oxygen was not concerned as a limiting substance of the system. The schematic diagram of the batch reactor is illustrated in Figure 4.1.

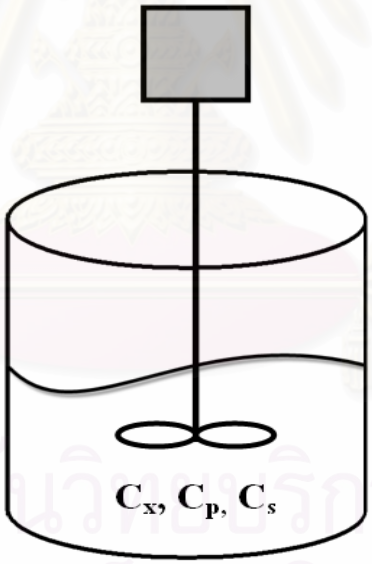

Figure 4.1 Schematic diagram of the batch reactor

The model could be written as:

$$\text{Cells:} \qquad \frac{dC_x}{dt} = \mu C_x - K_d C_x \qquad (4.1)$$

Ethanol: $$\frac{dC_p}{dt} = \nu C_x \qquad (4.2)$$

Substrate: $$-\frac{dC_s}{dt} = \frac{1}{Y'_{x/s}}\left(\frac{dC_x}{dt}\right) + \frac{1}{Y'_{p/s}}\left(\frac{dC_p}{dt}\right) + K_{CM} C_x \qquad (4.3)$$

The μ and ν were controlled by substrate limiting effect and inhibition effects of the substrate and ethanol as follows:

$$\mu = \mu_m \left(\frac{C_s}{K_s + C_s + \frac{C_s^2}{K_{SS}}} \right) \left(1 - \frac{C_p}{P_m} \right) \qquad (4.4)$$

$$\nu = \nu_m \left(\frac{C_s}{K_{SP} + C_s + \frac{C_s^2}{K_{SSP}}} \right) \left(1 - \frac{C_p}{P'_m} \right) \qquad (4.5)$$

where

K_{CM} maintenance constant (h^{-1})

K_d specific cell death rate (h^{-1})

K_S saturation growth constant (g/L)

K_{SP} saturation production constant (g/L)

K_{SS} substrate growth inhibition term (g/L)

K_{SSP} substrate production inhibition term (g/L)

P_m ethanol inhibition term for growth (g/L)

P'_m ethanol inhibition term for production (g/L)

C_P ethanol concentration (g/L)

C_{P0} initial ethanol concentration (g/L)

C_S substrate concentration (g/L)

C_{S0} initial substrate concentration (g/L)

C_X cell concentration (g/L)

C_{X0} initial cell concentration (g/L)

$Y'_{P/S}$ yield coefficient for product on substrate used for produce formation

$Y'_{X/S}$ yield coefficient for cells on substrate used for cell formation

μ specific growth rate (h^{-1})

μ_m maximum specific growth rate (h^{-1})

v specific production rate (h^{-1})

v_m maximum specific production rate (h^{-1})

For the process model considered, the operating time of the batch reactor is fixed to be 72 hour, and the temperature of fermentation is varied between 30 ^{0}C to 42 ^{0}C. Furthermore, the values of initial conditions of this process are described in Table 4.1.

Table 4.1 Initial conditions of the ethanol fermentation model

Initial conditions	Values (g/L)
C_{X0}	0.2
C_{P0}	0
C_{S0}	220

In ethanol fermentation processes, the temperature is one of the most important factors of the fermentation. Because temperature has strong effects on the kinetic parameters of ethanol fermentation. In this study, the influences of temperature on 12 kinetics parameters are described. Arrhenius relationships between operating temperature and the maximum specific growth rate, specific production rate, specific death rate are formulated. Polynomial equations are formulated for the effects of temperature on the other kinetic parameters. Table 4.2 displays the equations of the influence of temperature on 12 kinetics parameters.

Table 4.2 Equations of the influence of temperature on 12 kinetics parameters

Parameters	Equations
μ_m	$(3.10502*10^5)\ e^{-34,612/RT}$
ν_m	$(2.78329*10^6)\ e^{-34,345/RT}$
K_d	$(1.80091*10^{26})\ e^{-169,750/RT}$
K_s	$-0.07106267T^3 + 68.19059604T^2 - 21763.24255663T + 2310631.31257448$
K_{ss}	$0.25649202T^3 - 234.90430884T^2 + 71660.635582T - 7281204.58504586$
P_m	$0.14597513T^3 - 135.2839975T^2 + 41782.40344358T - 4300453.08856028$
K_{sp}	50
K_{ssp}	$1.7658799T^3 - 1634.4093777T^2 + 504125.732441T - 51819174.3601826$
P'_m	$0.1539499T^3 - 142.63999026T^2 + 44043.71451118T - 4532125.14105658$
$Y'_{X/S}$	$0.0005460616T^3 - 0.5060884977T^2 + 156.3141246493T - 16089.5995243401$
$Y'_{P/S}$	$-0.00005791656T^3 + 0.05534854016T^2 - 17.63089404155T + 1872.3739910691$
K_{CM}	0.03

where T = Temperature (Kelvin)

From Table 4.2 displays that the maximum specific growth rate (μ_m) and specific death rate (K_d) of cells and the maximum specific production rate of cells (ν_m) and saturation growth constant(K_S) increase as the temperature increases. The μ_m, K_d and ν_m are strongly depending on temperature in form of Arrhenius function.

However, these parameters such as K_{ss}, P_m, K_{ssp}, P'_m, $Y'_{X/S}$ and $Y'_{P/S}$ decrease as the temperature increases, whereas K_{sp} and K_{CM} are constant.

4.2 Optimal Temperature Control for Ethanol Fermentation in a Batch Reactor

Optimal temperature control strategy is used to determine the control temperature profile that satisfies the physical constraints and at the same time maximize (or minimize) performance criterion.

4.2.1 Problem Formulation

In the present study, an optimal temperature control problem related to ethanol fermentation in a batch reactor is studied. Maximum amount of desired ethanol product is studied to determine an optimal temperature profile of the fermentation. The obtained optimal temperature profile has to satisfy the specified objective function and other desired process constraints. Such optimal control problems can be described as follows.

4.2.1.1 Maximum Ethanol Fermentation Problem

Find the temperature T(t) over $t \in (t_0, t_f)$ for maximizing

$$J = C_P(t_f) \tag{4.6}$$

Subject to

$$\frac{dx}{dt} = f\left[x(t), u(t), t\right] \tag{4.7}$$

$$x(t_0) = x_0 \tag{4.8}$$

$$30^O C \le T(t) \le 42^O C \tag{4.9}$$

where t_f denotes the terminal time of the operation, $C_P(t_f)$ is the final ethanol concentration and J is the performance index which is the amount of the final ethanol product. Eq. (4.7) is the system of ordinary differential equations which are described by Eq. (4.1) through (4.3), Eq. (4.8) is the initial conditions for Eq. (4.7), Eqs. (4.9) is the upper and lower bounds on the temperature of the fermentation.

4.2.2 Simulation Results

In the current study, the sequential approach is applied for solving the optimal temperature control problems. Typically, a piecewise constant approximation over equally spaced time intervals is made for the control variables in the sequential approach.

4.2.2.1 Maximum Ethanol Fermentation

All simulation results given here are based on the optimal temperature control problem in the case of maximum ethanol fermentation. The objective is to find the optimal temperature profile which maximizes the amount of final ethanol product in the fixed operation time problem. The simulation results are classified into 2 cases.

Nominal Case

In the nominal case, the specified final batch time (t_f) is fixed at 72 hour, the batch length is divided in to 12 equal stages with equally spaced time interval of 6 hour and the control variable profiles are piecewise constant. The simulation results obtained from solving the optimal control problem by using the sequential approach are shown in Figures 4.2 and 4.3.

In Figure 4.2, the optimal temperature profile begins at 31.94 ^{0}C, then temperature decreases to approximately 30.38 ^{0}C. Finally, temperature increases again to approximately 31.26 ^{0}C. From the result, it could be described that in the first period, where the cell concentration is very low, in order to increases cell concentration, the optimal temperature profile begins with high temperature (31.94 ^{0}C). Then, the temperature is decreased to 30.38 ^{0}C. According to equation (4.1) in case of high cell concentration, term of cell death increases with the operating temperature. Therefore, the temperature is decreased to lower cell death rate. In the final period, cells are in stationary phase whereas the temperature is increased again around 31.26 ^{0}C for maximum ethanol production rate.

Figure 4.3 displays the ethanol, cell and sugar concentration profiles of the optimal temperature control system. At the end of the operation, the final ethanol concentration reaches 86.74 g/L, the final cell concentration is 6.91 g/L and the final sugar concentration is 37.52 g/L.

Optimization technique is also used to find the temperature of isothermal process which yields the maximum final ethanol concentration. The optimize temperature of isothermal process is 31.02 ^{0}C which yields final ethanol concentration of 86.63 g/L.

From the previous experimental reports by Torija et al. (2003), the temperature which yields maximum ethanol concentration by *Saccharomyces cerevisiae* was 30 ^{0}C. The final ethanol concentration at the isothermal process of 30 ^{0}C was reported at 83.34 g/L. Table 4.3 shows the final ethanol concentration from different processes.

Table 4.3 The final ethanol concentration at different processes

Processes	Final ethanol concentration (g/L)
Optimal temperature control	86.74
Isothermal 31.02 celcius (Optimization)	86.63
Isothermal 30 celcius (Torija et al.)	83.34

From Table 4.3 the optimal temperature control provides the best value of final ethanol concentration which demonstrates that the optimal temperature control technique assist the ethanol fermentation process operates effectively.

However, the final ethanol concentration of the optimal temperature control is only slightly higher than that of the isothermal 31.02 ^{0}C. This should be because of the narrow interval of the optimal temperature. With the limit of the optimal temperature range, the kinetic parameter values such as specific growth rate or specific production rate are slightly increased. Subsequently, the optimal temperature control yields the similarity of the system performance as the isothermal control.

Figure 4.4 shows cell concentration profile in the different processes. Cell concentration of the optimal temperature control is relative higher than that of the isothermal control in the first period due to the optimal temperature control begins with the higher temperature. In the second period, the cell concentration of the optimal temperature control is lower than the latter owing to the decreases of temperature to 30.38 ^{0}C. In the final period, the cell concentration of the optimal temperature control is again higher than that of the isothermal and the optimal temperature is slightly increased to 31.26 ^{0}C. Overall, after 72 hours of the fermentation, the final cell concentration in the system with the optimal control is slightly higher than that of the isothermal 31.02 ^{0}C.

Figure 4.5 displays the ethanol concentration profile in the different processes. In the first period, the ethanol concentration of the optimal temperature control is higher than that of the isothermal 31.02 ^{0}C because of the higher cell production from the operation at higher temperature. Since ethanol is a growth-associated product, ethanol production rate is related to the cell growth rate. In the second period, the ethanol concentration of the optimal temperature control is slightly lower than that of the isothermal 31.02 ^{0}C owing to the less ethanol production rate after the operating temperature is reduced. In the final period, the ethanol concentration of the optimal temperature control retains higher than that of the isothermal 31.02 ^{0}C due to the optimal temperature control has more cells to produce ethanol. Overall, after 72 hours of the fermentation, the cell concentration and ethanol concentration in the system with the optimal temperature control are relatively higher than those in the system with the isothermal 31.02 ^{0}C.

Effect of Time Interval

In previous section, the optimal temperature control problem is formulated as a fixed final time with equally spaced time interval of 6 hour. In this section, the effect of the time interval on the control performance is studied. The spaced time intervals are 3 hours and 1 hour.

Figure 4.7 displays the control response of the optimal temperature profiles computed using the time interval of 3 hours which shown in Figure 4.6. It is found that the final ethanol concentration obtained from the decreasing time is 86.7439 g/L which is slightly higher than that obtained in the nominal case.

Furthermore, Figure 4.8 shows the optimal temperature control profile using the time interval of 1 hour and Figure 4.9 displays the concentration profiles which obtained from the decreasing time interval to1 hour. It is found that the final ethanol concentration of 86.7451 g/L is obtained in the case of the time interval of

1 hour. The simulation results based on the optimal temperature control problem in the different time interval are summarized in Table 4.4.

Table 4.4 Comparison of the simulation results based on the optimal temperature control problem in the different time interval cases

Case studies	Final ethanol concentration (g/L)
The nominal case (time interval of 6 hour)	86.7360
The case of decreased time interval to 3 hours	86.7439
The case of decreased time interval to 1 hour	86.7451

From Table 4.4, it can be explained that at the length of time intervals decreases, the approximated optimal temperature profile with piecewise constant policy is closer to the actual optimal temperature profile (Shomchoam, 2006).

4.2.3 Conclusions

The optimal temperature control of a batch reactor for ethanol fermentation was studied in this work. The solution of the optimal temperature control problem was computed using a sequential approach. The optimal temperature control problem related to the ethanol fermentation process in a batch reactor (maximum ethanol fermentation) was considered. From the final ethanol concentration results at different processes it could be concluded that the optimal temperature control technique assists the ethanol fermentation process operates effectively in the similar performance as the isothermal one.

In addition, the effects of time interval were investigated in order to improve the control performance. From the simulation results, it could be concluded that the decreased time interval provides almost the same performance compared to the nominal case. Therefore, the nominal case (time interval of 6 hour) was used in further practice since it is more convenient for the operation than that of the decreasing time cases (time interval of 3 and 1 hour)

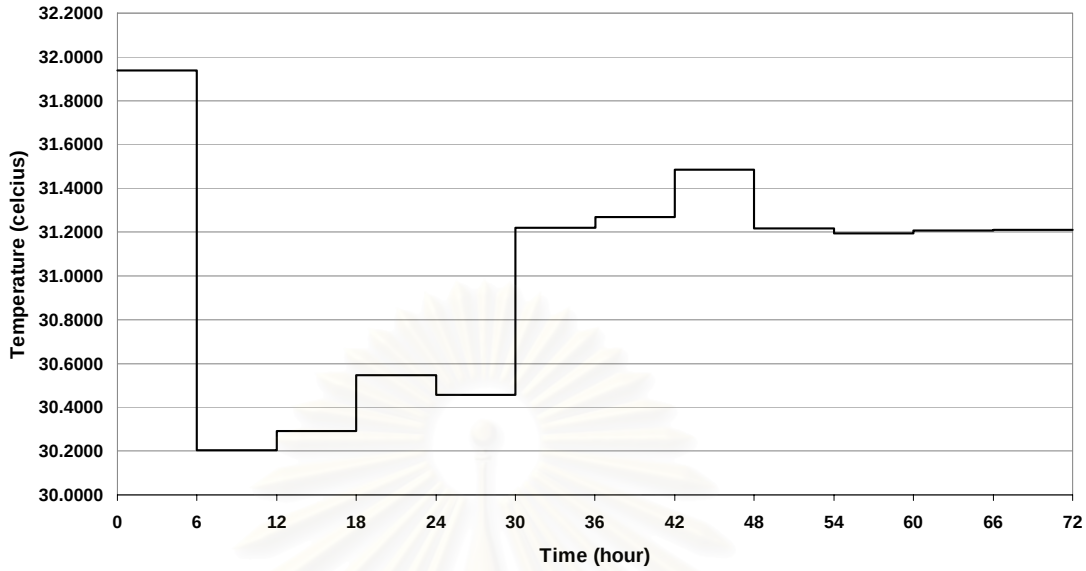

Figure 4.2 Optimal temperature profile in the nominal case

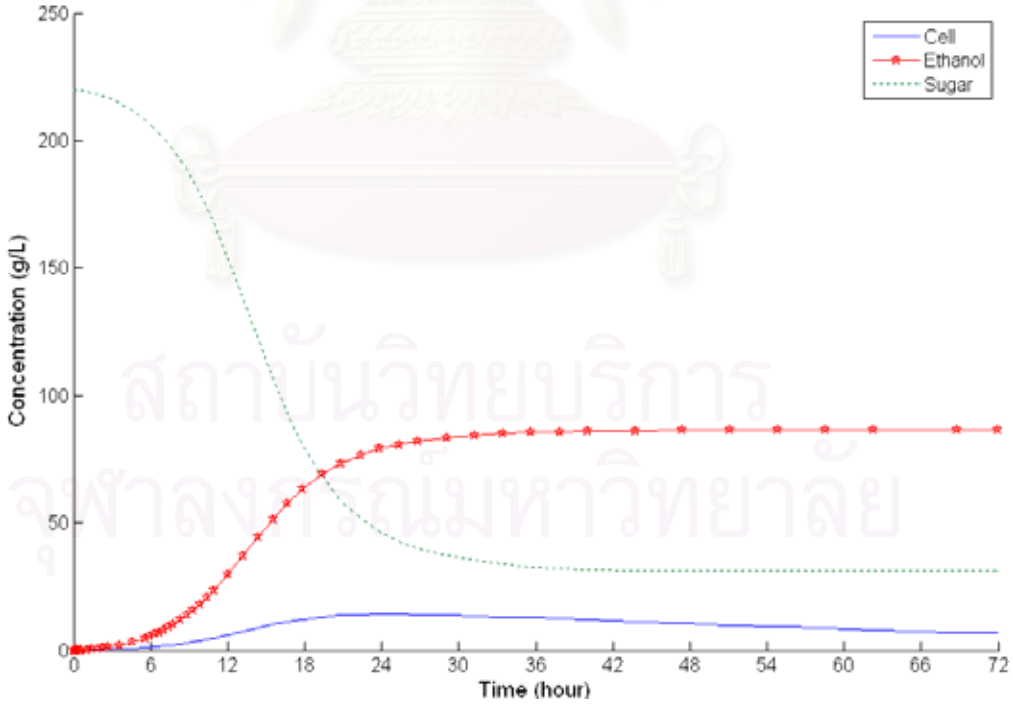

Figure 4.3 Concentration profile in the nominal case

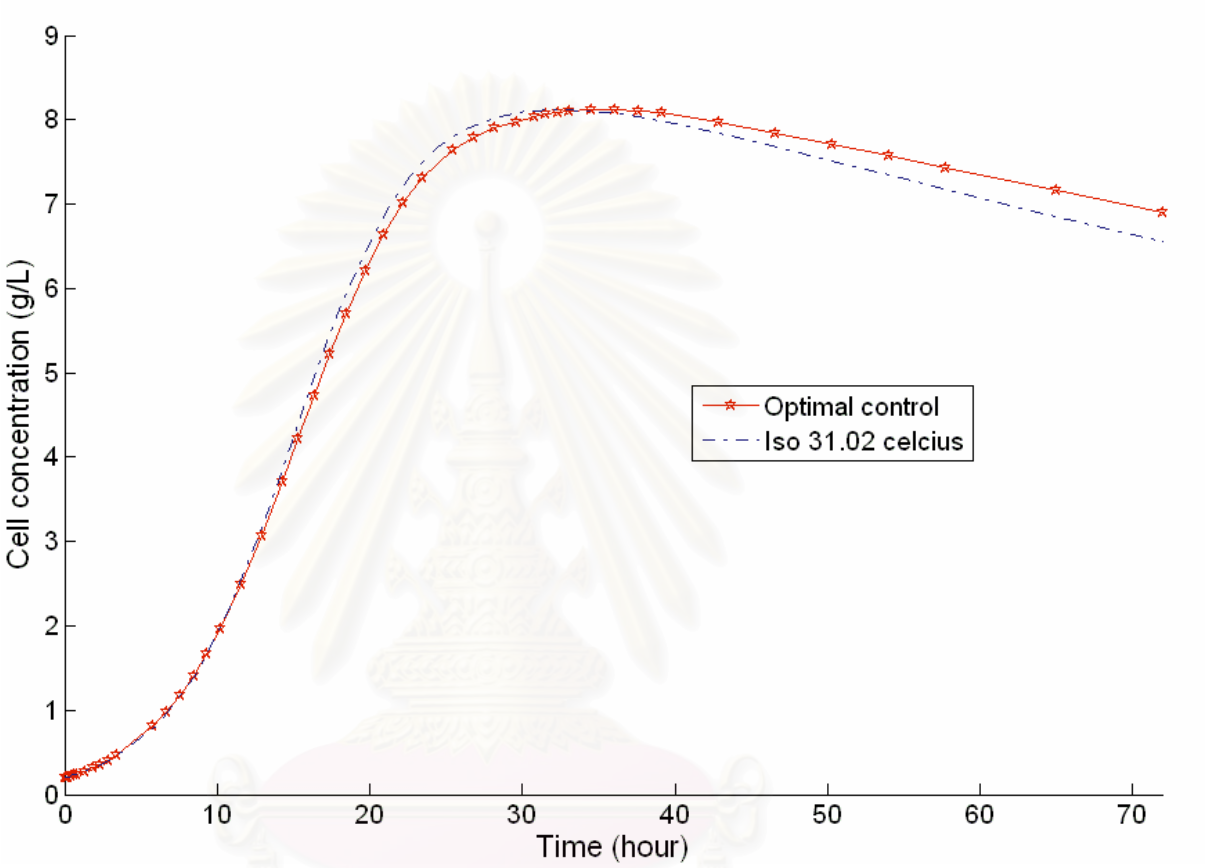

Figure 4.4 Cell concentration profile in the different processes

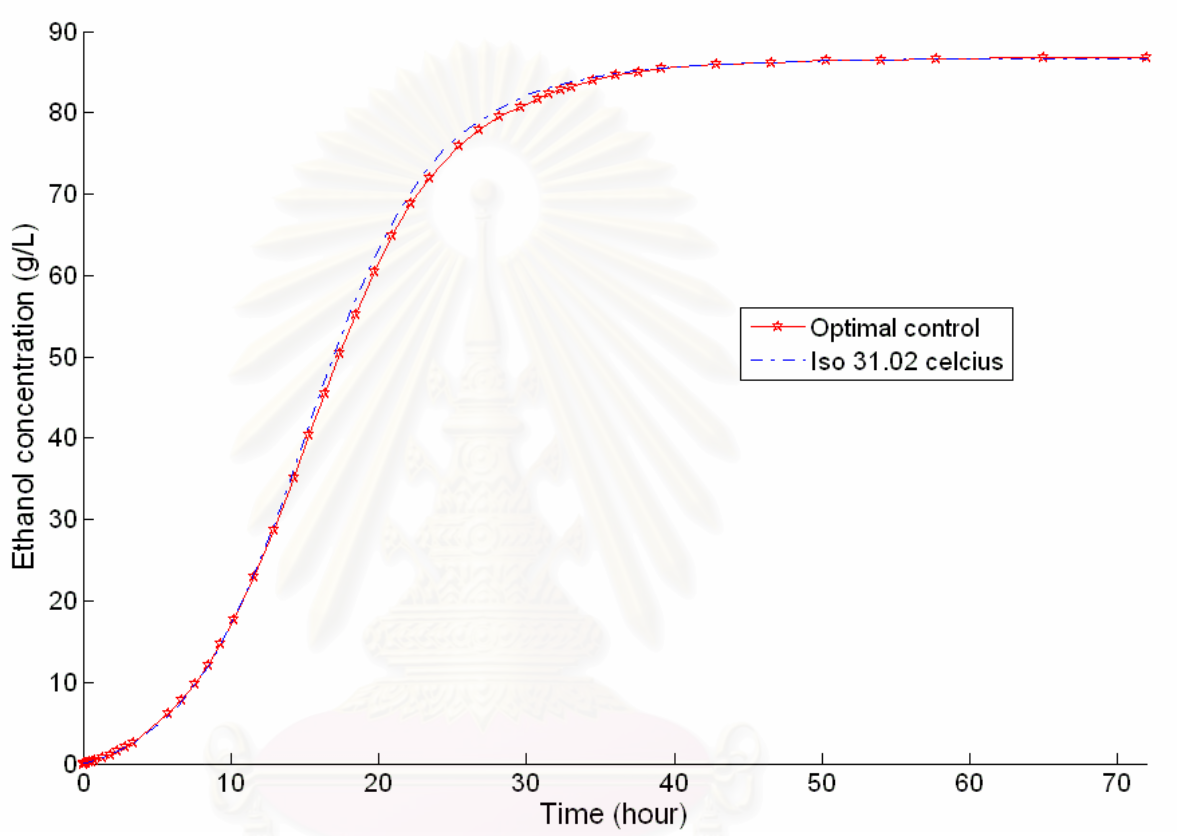

Figure 4.5 Ethanol concentration profile in the different processes

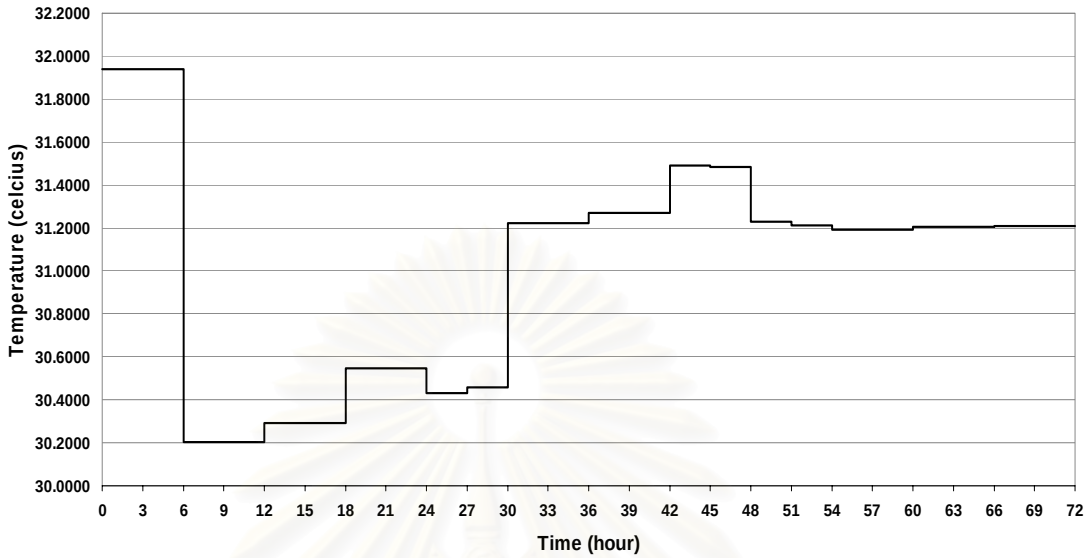

Figure 4.6 Optimal temperature profile in the case of decreased time interval (3 hr)

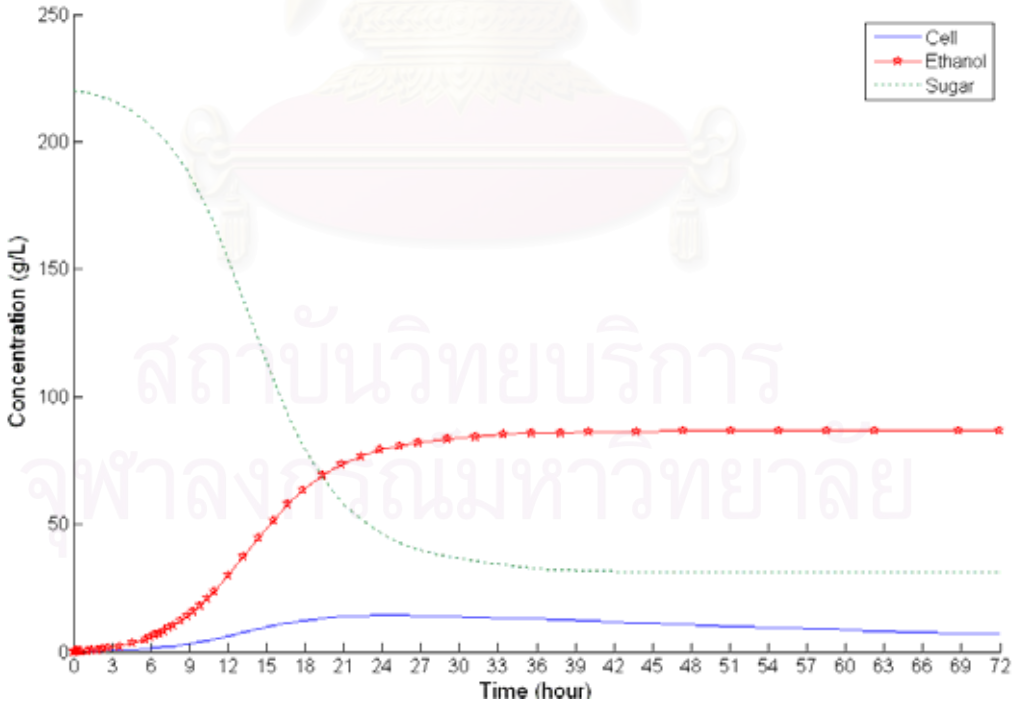

Figure 4.7 Concentration profile in the case of decreased time interval (3 hr)

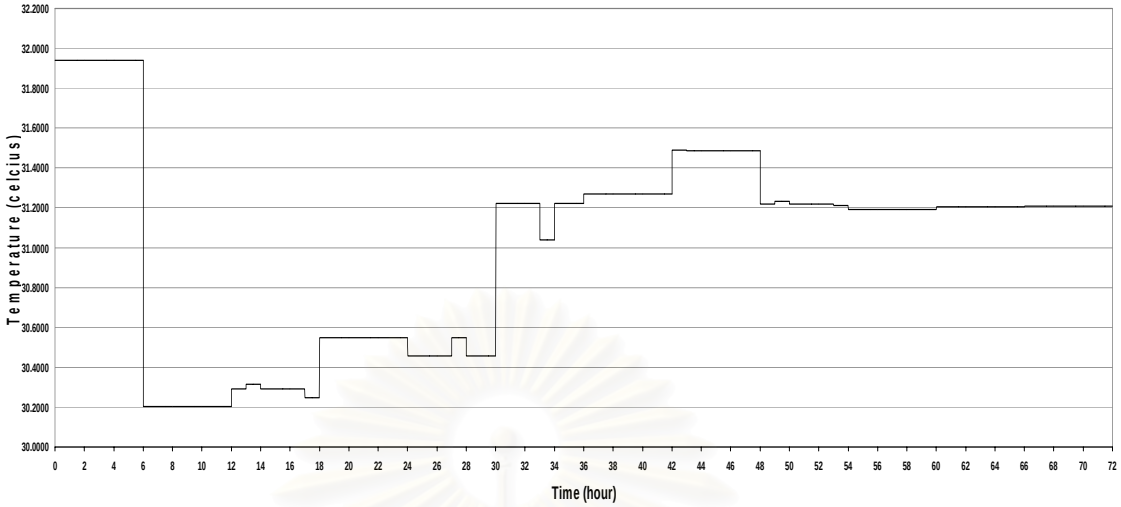

Figure 4.8 Optimal temperature profile in the case of decreased time interval (1 hr)

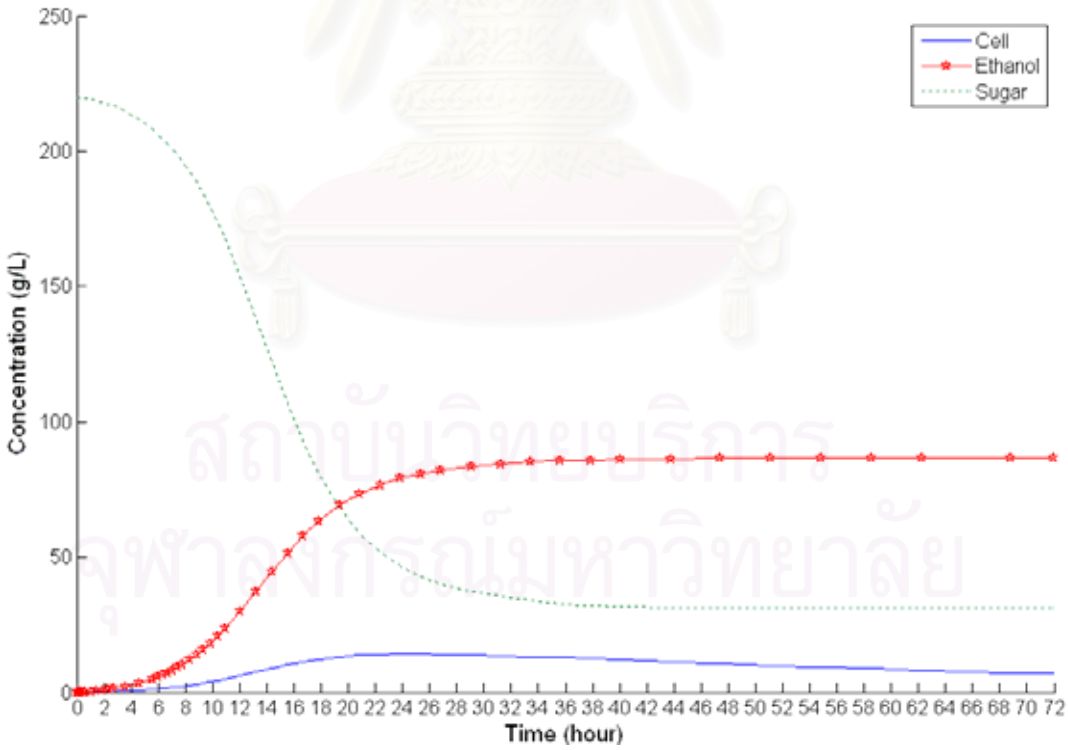

Figure 4.9 Concentration profile in the case of decreased time interval (1 hr)

CHAPTER V

PRELIMINARY ECONOMIC ANALYSIS

In this chapter, the preliminary economic analysis is employed to compare the results between the system with the optimal temperature control and the isothermal process. The preliminary economic analysis is considered on the operating cost of the process.

5.1 Description of Ethanol Production Process

The basic process flowsheet for ethanol production from molasses (Krajnc et. Al., 2006) is shown in Figure 5.1

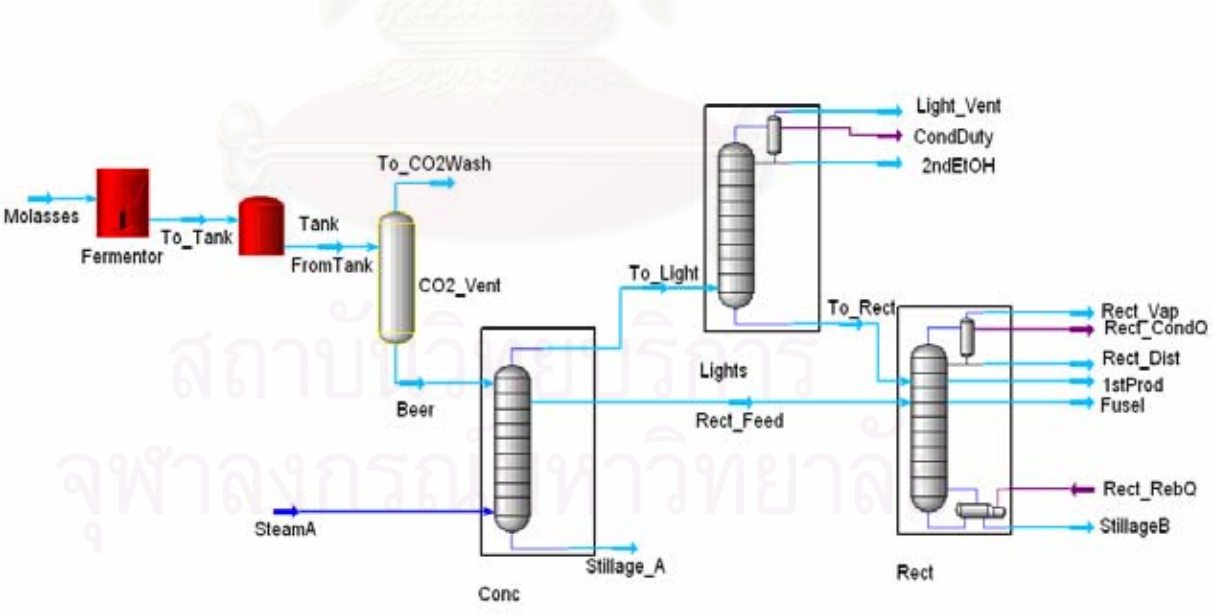

Figure 5.1 Process flowsheet for ethanol production from molasses

The elementary raw material in the process is molasses. It is thick, dark-colored syrup produced during sugar crystallization. At the beginning, the molasses is diluted with water to reduce its viscosity in the pipeline and is sterilized by direct steam injection. This stream is fed into the fermentation system.

After fermentation is finished, the fermentation beer is fed to the storage tank. The yeast precipitates to the bottom of tank. Carbon dioxide is produced during fermentation and it is separated from the ethanol in the absorber. The beer then flows into the section containing the distillation columns. Finally, the ethanol is removed from the mixture.

5.2 Preliminary Economic Analysis

Preliminary economic analysis is used to estimate the cost and profit of the process. These estimates provide the data necessary to evaluate the economic advantages of competing processes. The economic analysis of a process helps select and design process.

In this study, preliminary economic analysis on the operating cost is used to compare the results between the system with the optimal temperature control and the isothermal process (31.02^{o}C).

5.2.1 Productivity of Ethanol Production Process

In the present study, raw material is molasses. Molasses input rates of either the optimal temperature control or the isothermal process (31.02^{o}C) are 625 tons/day with the plant operating for 330 days/year (Yoosin et al., 2007). Molasses contain reducing sugar of 55 % weights by volume with the density of 1.2 g/cm^{3} (Royal Chitralada Projects, Bangkok, Thailand).

Table 5.1 Comparison of the ethanol productivity and ethanol conversion ratio of the system with optimal temperature control and isothermal process (31.02°C)

Item	Isothermal (31.02 °C)	Optimal temperature control
Molasses used (kg/year)	206,250,000	206,250,000
Ethanol yield (liter/year)	50,149,961	50,190,114
Ethanol conversion ratio (kg molasses/liter of ethanol)	4.1127	4.1094
Ethanol conversion yield (kg of ethanol/kg of molasses)	0.1918	0.1919

Table 5.1 shows the ethanol yield of the optimal temperature control in comparison to that of the isothermal (31.02 ^{0}C) based on molasses of 206,250 tons/year.

Table 5.2 displays the comparison of ethanol plant capacity and annual sales of the system with optimal temperature control and isothermal process (31.02°C)

Table 5.2 The comparison of ethanol plant capacity and annual sales of the system with optimal temperature control and isothermal process (31.02°C)

Item	Isothermal (31.02 °C)	Optimal temperature control
Ethanol capacity (liter/day)	151,969	152,091
Annual ethanol production (liter/year)	50,149,961	50,190,114
Annual sales (baht/year)	***777,324,410***	***777,946,768***

The average price of ethanol at ex-factory price is 15.5 baht per liter (ICIS pricing, 2007).

The results demonstrated that with the optimal temperature control strategy on the basis of 206,250 tons of molasses per year, the annual ethanol production is 40,152 liter/year or approximately 622,358 baht/year higher than those of the isothermal process (31.02^{o}C)

5.2.2 Operating Cost of Ethanol Production Process

In the current study, the operating expenses include molasses, steam, cooling water and wastewater treatment are estimated. Table 5.3 shows the comparison between the annual operating costs for the system with optimal temperature control and that of the isothermal process (31.02^{o}C).

In this study, the cost of steam is 0.42 baht/kg and cooling water is 0.000518 baht/kg (Yoosin et al., 2007) while, the adjusted cost of molasses to the year 2007 is 3.2 baht/kg (Gonsalves, 2006). In addition, the cost of wastewater treatment (activated sludge system) is 7.35 baht/m^3 (Industrial Estate Authority of Thailand, 2007).

Table 5.3 Annual operating cost comparison for the system with optimal temperature control and isothermal process (31.02^{o}C)

Cost factor	Annual cost (baht/year)	
	Isothermal (31.02 ^{o}C)	Optimal temperature control
Feedstocks (Molasses)	660,000,000	660,000,000
Utilities		
Steam	95,705,309	95,938,316
Cooling water	4,893,611	4,889,508
Wastewater treatment	3,249,901	3,248,599
Total annual operating cost	***763,848,821***	***764,076,423***

From Table 5.3, the total annual operating cost of the system with optimal temperature control is slightly higher than that of isothermal process (31.02°C). The feedstocks (Molasses) are major cost of total operating cost which conforms to the results of Yoosin (Yoosin et al., 2007).

Table 5.4 Operating cost comparison processing steps for the system with optimal temperature control and isothermal process (31.02°C)

Steps	Isothermal (31.02 °C)	Optimal temperature control
Raw materias (baht/year)	660,000,000	660,000,000
Fermentation (baht/year)	877,992	1,109,413
Separation (baht/year)	99,720,928	99,718,411
Wastewater treatment (baht/year)	3,249,901	3,248,599
Total (baht/year)	***763,848,821***	***764,076,423***

Table 5.4 displays the operating cost comparison processing steps for the system with the optimal temperature control and the isothermal process. Operating cost of fermentation step of the system with the optimal temperature control relatively higher than that of the isothermal process due to the temperature control strategy in the fermentation step. The system with the optimal temperature control requires both cooling water and steam for the temperature control, while the isothermal process uses only cooling water for the temperature control.

Meanwhile, the operating cost of separation step of the system with the optimal temperature control is rather lower than that of the latter process. Due to the higher final ethanol concentration, the required utilities for ethanol separation are less for the system with the optimal temperature control.

In addition, the operating cost for the wastewater treatment of the system with the optimal temperature control is slightly lower than that of the isothermal process owing to the less stillage effluents.

Overall, the total unit operating costs of the system with the optimal temperature control is relatively lower than that of the isothermal process. The details of the calculation are shown in Table 5.5.

Table 5.5 Unit operating cost comparison processing steps for the system with optimal temperature control and isothermal process (31.02^{o}C)

Steps	Isothermal (31.02 ^{o}C)	Optimal temperature control
Molasses (baht/liter of ethanol)	13.16	13.15
Fermentation (baht/liter of ethanol)	0.02	0.02
Separation (baht/liter of ethanol)	1.99	1.99
Wastewater treatment (baht/liter of ethanol)	0.06	0.06
Total (baht/liter of ethanol)	***15.23***	***15.22***

5.2.3 Profitability Analysis of Ethanol Production Process

To be a worthwhile investment, a venture for the installation of a new chemical plant or a revamp of an existing plant must be profitable. Therefore, the profitability analysis is used to evaluate the economic advantages of competing projects.

In the present study, the annual profit of ethanol production process is calculated from equation (5.1). Table 5.6 displays the annual profit comparison for the system with optimal temperature control and isothermal process (31.02^{o}C).

The annual profit = The annual sales – The total annual operating cost (5.1)

Table 5.6 Annual profit comparison for the system with optimal temperature control and isothermal process (31.02°C)

Item	Isothermal (31.02 °C)	Optimal temperature control
Annual sales (baht/year)	777,324,410	777,946,768
Total annual operating cost (baht/year)	763,848,821	764,076,423
Annual profit (baht/year)	***13,475,589***	***13,870,345***

Table 5.6 demonstrates that the annual profit of the system with optimal temperature control is relatively higher than that of isothermal process. Table 5.7 displays the unit profit comparison for the system with optimal temperature control and isothermal process. Overall, the unit profit of the system with optimal temperature control is slightly higher than that of the latter one.

Table 5.7 Unit profit comparison for the system with optimal temperature control and isothermal process (31.02°C)

Item	Isothermal (31.02 °C)	Optimal temperature control
Sales (baht/liter of ethanol)	15.50	15.50
Operating cost (baht/liter of ethanol)	15.23	15.22
Profit (baht/liter of ethanol)	***0.27***	***0.28***

5.2.4 Conclusions

In this chapter, preliminary economic analysis on the operating cost was used to compare the results between the system with the optimal temperature control and the isothermal process (31.02^{o}C). The results showed that the ethanol capacity, annual ethanol production and annual sales of the system with the optimal temperature control were relatively higher than those of the isothermal process.

With the optimal control strategy, the total annual operating cost of the system was rather higher whereas the unit operating cost was relatively lower than that of the isothermal process.

In addition, the annual and unit profit of the system with the optimal temperature control was to a certain extent higher than that of the isothermal process. From these results demonstrated that the optimal temperature control technique assist the ethanol fermentation process operates effectively.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

Presently, the Thai government has an intention to substitute the imported crude oil by indigenous resources of bio-fuel. The primary purpose of the Thai government is to promote ethanol as a substitute fuel for gasoline octane 95. Hence, the price competitiveness between them is one of the most important factors that the government is concerned about.

The total production cost of ethanol can be reduced by operating the ethanol fermentation process effectively. Therefore, the optimal control strategy for controlling temperature of a batch reactor can be applied to improve the ethanol fermentation process.

In this research, the temperature control of the ethanol fermentation process in a batch reactor was studied. The optimal temperature control strategy was applied to obtain the maximum amount of the desired ethanol product at the end of the operation.

In the optimal temperature control technique, the solution of the optimal temperature control problem was computed using a sequential approach. The results showed that the optimal temperature control provided the best value of final ethanol concentration among other processes.

In addition, the effects of time interval were investigated in order to improve the control performance. From the simulation results, it could be seen that decreasing the time interval provided a slightly better control performance compared to the nominal case. However, the nominal case (time interval of 6 hours) was used in practice because of the more convenient adjustment of temperature.

Finally, preliminary economic analysis on the operating cost was used to compare the results between the system with the optimal temperature control and the isothermal process (31.02^{o}C). The results displayed that the unit operating costs of the system with the optimal temperature control was relatively lower than that of the isothermal process and the unit profit of the system with the optimal temperature control was to some extent higher than that of the isothermal process. These results demonstrated that the optimal temperature control technique assist the ethanol fermentation process operates effectively.

6.2 Recommendations

According to this work, the optimization technique which the performance index is the operating cost of ethanol production is recommended to find the isothermal temperature that minimizes the operating cost.

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APPENDICES

APPENDIX A

THE ESTIMATION OF UTILITY COST

A.1 The Estimation of Utility Cost in Fermentor

In this research, the fermentors are divided to 2 types.

A.1.1 Isothermal Fermentor

In the isothermal fermentor, the energy balance is unsteady-state nonisothermal which developed from the general energy balance (Fogler, 1999)

Rate of accum. of energy within system	=	Rate of flow of heat to system from surrounding	-	Rate of work done by system on surrounding	+	Rate of energy added to system by mass flow into system	-	Rate of energy leaving system by mass flow out system

$$\frac{d\hat{E}_{sys}}{dt} = \dot{Q} - \dot{W} + \sum_{i=1}^{n} F_0 E_0 - \sum_{i=1}^{n} F_i E_i \quad \text{(A.1)}$$

When shear stresses are absent

$$\dot{W} = - \sum_{i=1}^{n} F_0 PV_0 + \sum_{i=1}^{n} Fi PV_i + \dot{W}_s \quad \text{(A.2)}$$

where P is the pressure and V is the specific volume and $\dot{W}_s$ is the shaft work

Substitute Eq. (A.2) into Eq. (A.1) and grouping terms gives

$$\frac{d\hat{E}_{sys}}{dt} = \dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_{i0}(E_{i0} + PV_{i0}) - \sum_{i=1}^{n} F_i(E_i + PV_i) \quad \text{(A.3)}$$

and set $E_i = U_i$ (A.4)

From $H_i = U_i + PV_i$ (H_i = enthalpy) (A.5)

Combining Eq. (A.3), (A.4) and (A.5) gives

$$\frac{d\hat{E}_{sys}}{dt} = \dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_{i0}H_{i0} - \sum_{i=1}^{n} F_{i0}H_i \quad \text{(A.6)}$$

Set $\hat{E}_{sys} = \sum_{i=1}^{n} N_i E_i$ (A.7)

Differentiating Eq. (A.7) and substitute into Eq. (A.6) gives

$$\dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_{i0}H_{i0} - \sum_{i=1}^{n} F_{i0}H_i = \sum_{i=1}^{n} N_i \frac{dH_i}{dt} + \sum_{i=1}^{n} H_i \frac{dN_i}{dt} \quad \text{(A.8)}$$

From $H_i = H^0(T_R) + \int C_{pi}\,dT$ (A.9)

Differentiating Eq. (A.9) and substitute into Eq. (A.8) gives

$$\dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_{i0}H_{i0} - \sum_{i=1}^{n} F_{i0}H_i = \sum_{i=1}^{n} N_i C_{pi} \frac{dT}{dt} + \sum_{i=1}^{n} H_i \frac{dN_i}{dt} \quad \text{(A.10)}$$

The mole balance on species i is

$$\frac{dN_i}{dt} = - \nu_i r_A + F_{i0} - F_i \qquad \text{(A.11)}$$

Using Eq. (A.11) to substitute into Eq. (A.10) and rearranging gives

$$\sum_{i=1}^{n} N_i C_{pi} \frac{dT}{dt} = \dot{Q} - \dot{W}_s - \sum_{i=1}^{n} F_{i0} C_{pi} (T-T_{i0}) + [-\Delta H_{Rx}](-r_A V) \qquad \text{(A.12)}$$

In the batch reactor, F_{i0} equal to zero and neglects $\dot{W}_s$ Eq. (A.12) yielding

$$\sum_{i=1}^{n} N_i C_{pi} \frac{dT}{dt} = \dot{Q} + [-\Delta H_{Rx}](-r_A V) \qquad \text{(A.13)}$$

In the isothermal fermentor Eq. (A.13) yielding

$$\dot{Q} = [(\Delta H_{Rx})(-r_A)](V) \qquad \text{(A.14)}$$

In this research set $[(\Delta H_{Rx})(-r_A)] = r_Q$

which $r_Q = 467.8\, r_S - 463.9\, r_x - 684.5\, r_p$ (A.15)

where r_Q = volumetric heat production rate (kJ/(m^3 h))

r_S = rate of consumption of substrate (kg/(m^3 h))

r_x = rate of production of cells (kg/(m^3 h))

r_p = rate of production of ethanol (kg/(m^3 h))

and the Eq. (A.15) is formulated from Turker's research (Turker, 2004) thus Eq. (A.14) becomes

$$\dot{Q} = (r_Q)\ (V) \qquad \text{(A.16)}$$

From Eq. (A.16) can calculate heat of the isothermal fermentor and then estimate utility cost. The volumetric heat production rate of the system with the isothermal 31.02 ^{0}C is calculated and presented in Figure A.1

A.1.2 Nonisothermal Fermentor

From the optimal temperature control which is applied for control temperature of fermentor, the temperature in fermentor is nonisothermal thus the energy balance is Eq. (A.13) and set $[(\Delta H_{Rx})(-r_A)] = r_Q$ gives

$$\dot{Q} = \sum_{i=1}^{n} N_i C_{pi} \frac{dT}{dt} + [(r_Q)\ (V)] \qquad \text{(A.17)}$$

From Eq. (A.17) can calculate heat of the nonisothermal fermentor and then estimate utility cost. The volumetric heat production rate of the system with the optimal temperature control is calculated and shown in Figure A.2.

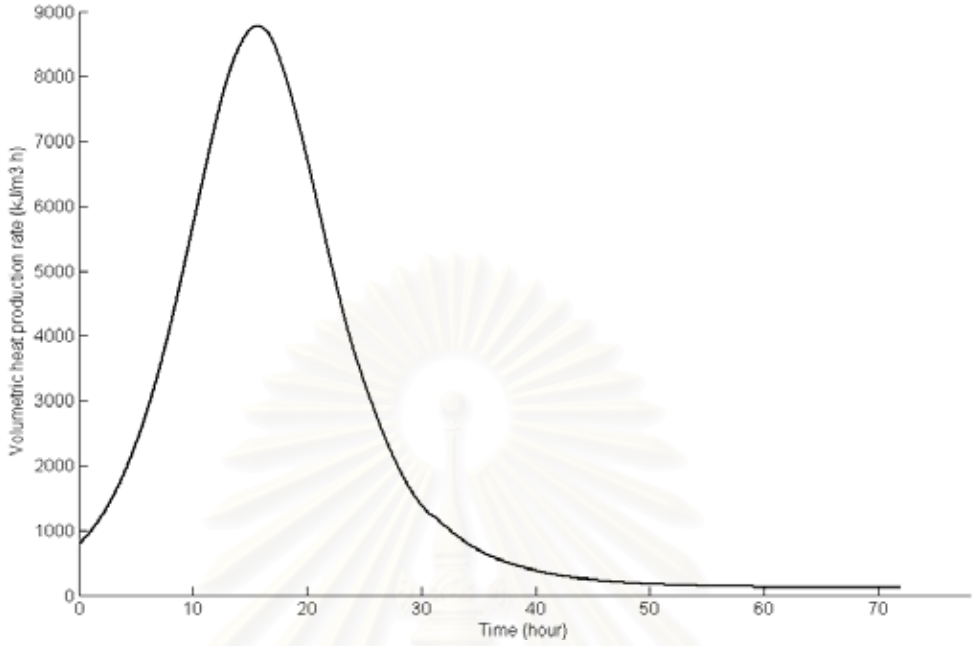

Figure A.1 The volumetric heat production rate of the system with the isothermal 31.02 ^{0}C

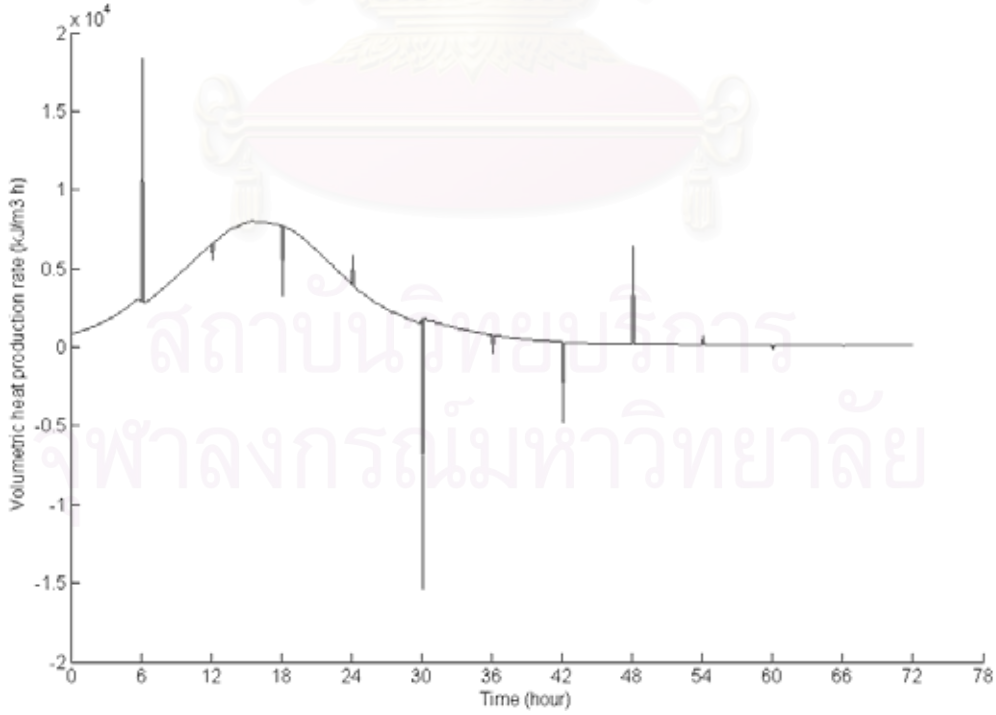

Figure A.2 The volumetric heat production rate of the system with the optimal temperature control

A.2 The Estimation of Utility Cost in Separation Step

In this study, the system with the optimal temperature control and the isothermal 31.02 ^{0}C use same process which is shown in Figure 5.1. The material streams of process flowsheet from HYSYS simulation are displayed in Table A.1 and Table A.2.

Table A.1 Material streams of the system with the optimal temperature control

Name	FromTank	SteamA	To_CO2Wash
Vapour Fraction	0.040	1.000	1.000
Temperature [C]	30.000	140.000	30.000
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	2864.500	610.599	114.713
Mass Flow [kg/h]	59018.453	11000.000	4933.382
Liquid Volume Flow [m3/h]	61.289	11.022	5.965
Heat Flow [kJ/h]	-823763361.853	-144764682.691	-44039175.664

Name	Beer	To_Light	Stillage_A
Vapour Fraction	0.000	1.000	0.000
Temperature [C]	30.000	84.948	99.992
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	2749.787	12.318	3091.400
Mass Flow [kg/h]	54222.670	380.198	57352.258
Liquid Volume Flow [m3/h]	55.324	0.445	57.199
Heat Flow [kJ/h]	-779724186.188	-3121052.447	-860907510.124

Name	Rect_Feed	Light_Vent	2ndEtOH
Vapour Fraction	1.000	1.000	0.000
Temperature [C]	88.082	34.380	34.380
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	256.668	1.600	4.162
Mass Flow [kg/h]	7490.213	69.584	161.754
Liquid Volume Flow [m3/h]	8.702	0.084	0.198
Heat Flow [kJ/h]	-60460159.656	-596969.329	-1160040.231

Name	To_Rect	Rect_Vap	Rect_Dist
Vapour Fraction	0.000	1.000	0.000
Temperature [C]	80.584	78.032	78.032
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	6.556	0.100	0.047
Mass Flow [kg/h]	148.860	4.304	2.000
Liquid Volume Flow [m3/h]	0.162	0.005	0.002
Heat Flow [kJ/h]	-1827806.469	-23255.406	-12618.221

Name	StillageB	1stProd	Fusel
Vapour Fraction	0.000	0.000	0.000
Temperature [C]	99.998	78.106	83.835
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	145.956	116.989	0.133
Mass Flow [kg/h]	2629.409	**5000.360**	3.000
Liquid Volume Flow [m3/h]	2.635	6.218	0.003
Heat Flow [kJ/h]	-40753125.684	-31714972.519	-37031.219

Table A.2 Material streams of the system with the isothermal 31.02 ^{0}C

Name	FromTank	SteamA	To_CO2Wash
Vapour Fraction	0.040	1.000	1.000
Temperature [C]	30.000	140.000	30.000
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	2866.000	610.599	114.721
Mass Flow [kg/h]	59020.054	11000.000	4933.689
Liquid Volume Flow [m3/h]	61.320	11.022	5.966
Heat Flow [kJ/h]	-825594792.744	-144764682.691	-44042426.975

Name	Beer	To_Light	Stillage_A
Vapour Fraction	0.000	1.000	0.000
Temperature [C]	30.000	84.935	99.984
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	2755.279	12.357	3096.864
Mass Flow [kg/h]	54233.005	381.398	57364.203
Liquid Volume Flow [m3/h]	55.244	0.446	58.187
Heat Flow [kJ/h]	-781552365.769	-3131875.979	-862725270.572

Name	Rect_Feed	Light_Vent	2ndEtOH
Vapour Fraction	1.000	1.000	0.000
Temperature [C]	88.083	33.508	33.508
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	256.657	1.600	4.182
Mass Flow [kg/h]	7487.405	69.625	162.568
Liquid Volume Flow [m3/h]	8.698	0.085	0.199
Heat Flow [kJ/h]	-60458235.568	-598554.795	-1166320.489

Name	To_Rect	Rect_Vap	Rect_Dist
Vapour Fraction	0.000	1.000	0.000
Temperature [C]	80.585	78.032	78.032
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	6.575	0.100	0.047
Mass Flow [kg/h]	149.205	4.304	2.000
Liquid Volume Flow [m3/h]	0.162	0.005	0.002
Heat Flow [kJ/h]	-1833009.801	-23254.807	-12617.785

Name	StillageB	1stProd	Fusel
Vapour Fraction	0.000	0.000	0.006
Temperature [C]	99.998	78.106	83.979
Pressure [kPa]	101.325	101.325	101.325
Molar Flow [kgmole/h]	146.072	116.880	0.133
Mass Flow [kg/h]	2631.494	**4995.812**	2.998
Liquid Volume Flow [m3/h]	2.637	6.213	0.003
Heat Flow [kJ/h]	-40785444.805	-31685407.203	-37111.921

The energy streams of process flowsheet from HYSYS simulation are displayed in Table A.3 and Table A.4. Then estimate utility cost from these energy streams.

Table A.3 Energy streams of the system with the optimal temperature control

Name	CondDuty	Rect_RebQ	Rect_CondQ
Heat Flow [kJ/h]	463771.2385	30197757.39	40449618.42

Table A.4 Energy streams of the system with the isothermal 31.02 ^{0}C

Name	CondDuty	Rect_RebQ	Rect_CondQ
Heat Flow [kJ/h]	466032.8235	30199003.36	40448145.09

VITA

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