MODELING AND SIMULATE ALCOHOL FERMENTATION PROCESS BY SIMULINK

MÔ HÌNH HOÁ VÀ MÔ PHỎNG QUÁ TRÌNH LÊN MEN CỒN TRÊN SIMULINK

Tran Van Tai, Nguyen Truong Giang, Nguyen Duc Trung*

ABSTRACT

Ethanol fermentation is widely used in the production of foods like alcoholic beverages. In previous research, the production of ethanol by batch fermentation and continuous fermentation process was examined. Continuous fermentation is a complex process consisting of many alterations of energy and matter flows. For improving the overall fermentation process efficiency, a rigorous analysis to determine optimal values for operation variables is needed. Simulation of the process is a recognized way for doing such an analysis. In this study, a MIMO (Multi Input, Multi Output) nonlinear multivariable predictive controller was developed for an alcoholic fermentation process. Effect of agitation rate and heat exchange in bioreactors during ethanol fermentation wasn't analyzed. Mathematical models were used to predict the influence of operating parameters on cell concentration, substrate utilization rate and ethanol production rate. The basic principle used in this model is a concept of balance theory of mass and energy.Parameter were estimated from experimental data. The kinetic model with its parameters was applied in the simulation of a continuous fermentation process for ethanol production. Simulations for multiple scenarios were carried out using software tool Simulink using block diagrams, overlaid on the Matlab R2016a programming language. Results was obtained in the simulation is the basis for the preliminary evaluation of results in optimization, identification and linearization and can be used for design of the control systems as well as the operating mode prediction.

Keywords: *Continuous ethanol fermentation process; dynamic simulation; kinetic model; MIMO; Simulink.*

TÓM TẮT

Hệ thống lên men cồn được ứng dụng nhiều trong công nghiệp thực phẩm. Các nghiên cứu về chúng thường là khảo sát các hệ thống lên men gián đoạn (theo mẻ) hoặc liên tục, quá trình lên men liên tục được mô hình hóa động học và mô phỏng trong nghiên cứu này. Đây là một quá trình phức hợp gồm nhiều quá trình biến đổi của các dòng năng lượng và dòng vật chất. Quá trình lên men liên tục được nhìn nhận với tư cách một đối tượng điều khiển là một mô hình động học phi tuyến đa biến với các tương tác chéo của các tín hiệu vào và các tín hiệu ra (hệ đa biến - MIMO). Quá trình khuấy trộn và quá trình truyền nhiệt không được tập trung đi sâu phân tích trong nghiên cứu. Mô hình hóa động học được xây dựng chi tiết làm cơ sở cho mô phỏng quá trình lên men liên tục. Cân bằng năng lượng và cân bằng vật chất là hai nguyên lý căn bản được sử dụng trong mô hình hóa. Thiết kế mô phỏng dựa trên công cụ đồ hình của phần mềm Simulink được đóng trong gói Matlab R2016a. Kết quả của các trường hợp hoạt động sản xuất khác nhau có thể được đưa ra từ sơ đồ mô phỏng này. Đây là cơ sở cho việc đánh giá sơ bộ các kết quả nghiên cứu về tối ưu, nhận dạng và tuyến tính hóa phục vụ thiết kế hệ thống điều khiển hệ thống cũng như dự báo chế độ vận hành.

Từ khóa: *Lên men liên tục, mô phỏng động học, mô hình động học, MIMO, Simulink.*

Hanoi University of Science and Technology
*Email: trung.nguyenduc@hust.edu.vn
Received: 25/4/2021
Revised: 05/6/2021
Accepted: 25/6/2021

1. INTRODUCTION

Fermentation is a key process stage in ethanol production. For improving the cost efficiency, production efficiency and obtaining desired product, the research to optimize the fermentation process for defining the best operating parameters is needed. Fermentation is a multivariable control system with complex nonlinear kinetics [1]. There are multiple modeling methods but with complex technical systems models, the nonlinear system of differential equations often used. Simulation and optimization of fermentation conditions for the production of ethanol has gained great importance in the manufacturing practice. Effective and reliable assessment utility for continuous alcohol fermentation process was established in this study.

In the mathematical model used in simulation, in addition to the detailed kinetics model also includes computational equations describing heat transfer, temperature dependence of kinetic parameters, oxygen transfer as well as the effect of metal concentration and temperature on mass transfer. The kinetic equations used in the mentioned bioreactor model are modifications of the Monod equations based on the Michaelis–Menten kinetics, proposed by Aiba.

2. A STATE - SPACE MODEL FOR AN ALCOHOLIC FERMENTATION

In this study, the spatial distribution of parameters in the bioreactor wasn't assessed. The quantities were referred to the concentrated parameters

mathematical model based on the model assumption of uniform distribution (ideal stirred tank) [2].

Ethanol production is divided into two phases: respiration (yeast propagation under aerobic conditions) and ethanol fermentation under anaerobic conditions:

- Aerobic conditions: $C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$
- Anaerobic conditions: $C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2\ CO_2 + Q$

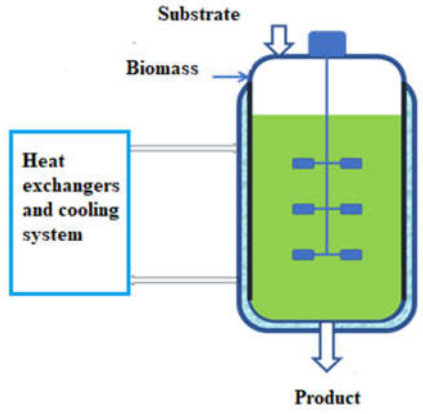

Figure 1. Flow diagram of transform matter in bioreactor

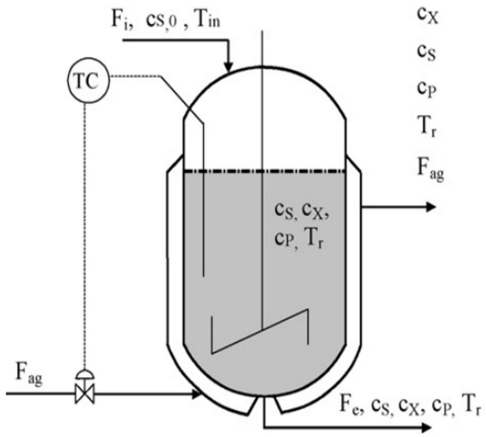

Figure 2. The continuous fermentation reactor

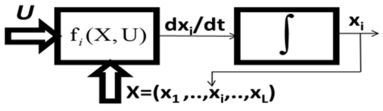

Figure 3. Diagram description of a state variable x_i

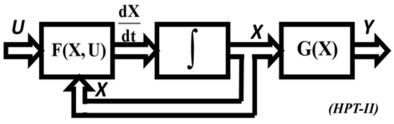

Figure 4. Diagram description of the system state equation

The continuous fermentation reactor is shown in Fig. 1 and 2 described as a block diagram of the input (U) and output (Y) vectors. Dynamic response in output Y to step change in input U (Fig. 4).

$$\begin{cases} \dfrac{dX}{dt} = F(X,U) \\ Y = G(X,U) \end{cases} \xrightarrow{i=\overline{1,n}} \frac{dx_i}{dt} = f_i(X,U) \quad (I)$$

The bioreactor is modeled as a continuous stirred tank with constant the substrate flow. There is also a constant outlet flow from the bioreactor that includes the product, substrate and biomass (Fig. 2).

The kinetic equations used in the mentioned bioreactor model are modifications of the Monod equations based on the Michaelis-Menten kinetics, proposed by Aiba et al [3].

$$\frac{dc_X}{dt} = \mu_X c_X \frac{c_S}{K_S + c_S} e^{-K_p c_p} \quad (1)$$

$$\frac{dc_P}{dt} = \mu_P c_X \frac{c_S}{K_{S1} + c_S} e^{-K_{p1} c_p} \quad (2)$$

$$\frac{dc_S}{dt} = \frac{1}{R_{SX}} \frac{dc_X}{dt} - \frac{1}{R_{SP}} \frac{dc_P}{dt} \quad (3)$$

Where R_{SX} and R_{SP} are defined asratio of cell produced per glucose consumed for growth and ratio of ethanol produced per glucose consumed for fermentation, respectively.

Inorganic salts are added with the yeast. Those are necessary compounds for the formation of coenzymes. But the inorganic salts also have a strong effect on the equilibrium concentration of oxygen in the liquid phase.

Effect of the ionic concentration is calculated by Eq (4):

$$\sum H_i I_i = H_{Na} I_{Na} + H_{Ca} I_{Ca} + H_{Mg} I_{Mg} + H_{Cl} I_{Cl} + H_{CO_3} I_{CO_3} + H_H I_H + H_{OH} I_{OH} = 0{,}1274 \quad (4)$$

The equilibrium concentration of oxygen depend on temperature in distilled water is given by the empirical equation as follows [4] :

$$c^*_{O_2,0} = 14.6 - 0.3943T_r + 0.007714T_r^2 - 0.0000646T_r^3 \quad (5)$$

In the fact that salts are dissolved in the medium the equilibrium concentration of oxygen in liquid phase is calculated by Setchenov equation [4]:

$$c^*_{O_2} = c^*_{O_2,0} \times 10^{-\sum H_i I_i} \quad (6)$$

Mass transfer coefficient for oxygen related to temperature is determined by the following empirical equation [5]:

$$(k_l a) = (k_l a)_0 (1.024)^{T_r - 20}$$

Equation for the rate of oxygen consumption is:

$$r_{O_2} = \mu_{O_2} \frac{1}{Y_{O_2}} c_X \frac{c_{O_2}}{K_{O_2} + c_{O_2}} \quad (7)$$

The formula of the maximum specific growth rate related to the growth rate that increases with the temperature and the effect of the heat denaturation:

$$\mu_X = A_1 e^{-(E_{a1}/R(T_r+273))} - A_2 e^{-(E_{a2}/R(T_r+273))} \quad (8)$$

In continuous fermentation process, there are inlet and outlet flow. Total volume of the reaction medium is:

[Rate of change in volume] = [Volume input rate] – [Volume output rate]

$$\frac{dV}{dt} = F_i - F_e \quad (9)$$

Where: F_i and F_e are defined as flow of substrate entering the reactor and outlet flow from the reactor, respectively.

A biomass balance is presented as follows:

$$\frac{dc_X}{dt} = \mu_X c_X \frac{c_S}{K_S + c_S} e^{-K_p c_p} - \frac{Fe}{V} c_X \quad (10)$$

The mass balance for the product is presented by the following equation:

$$\frac{dc_P}{dt} = \mu_P c_X \frac{c_S}{K_{S1} + c_S} e^{-K_{p1} c_p} - \frac{Fe}{V} c_P \quad (11)$$

A substrate mass balance is expressed by Eq. (12):

[Substrate utilization rate] = [Substrate input rate] – [Substrate output rate] – [Substrate uptake rate for growth] – [Substrate uptake for production formation]

$$\frac{dc_S}{dt} = -\frac{1}{R_{SX}} \mu_X c_X \frac{c_S}{K_S + c_S} e^{-K_p c_p} + \frac{Fi}{V} c_{S,in} - \frac{1}{R_{SP}} \mu_P c_X \frac{c_S}{K_{S1} + c_S} e^{-K_{p1} c_p} - \frac{Fe}{V} c_S \quad (12)$$

The concentration of the dissolved oxygen in the reaction medium is calculated by Eq.(13):

[Oxygen utilization rate] = [Oxygen input rate due to the mass transfer] – [Oxygen rate consumed for fermentation reaction]

$$\frac{dc_{O_2}}{dt} = (k_l a)(c^*_{O_2} - c_{O_2}) - r_{O_2} \quad (13)$$

An energy balance for the fermentation process is given as below:

For the bioreactor:

$$\frac{dT_r}{dt} = \frac{F_i}{V}(T_{in} + 273) - \frac{F_e}{V}(T_r + 273) + \frac{r_{O_2} \Delta H_r}{32 \rho_r C_{heat,r}} + \frac{K_T A_T (T_r - T_{ag})}{V \rho_r C_{heat,r}} \quad (14)$$

For the jacket:

$$\frac{dT_{ag}}{dt} = \frac{F_{ag}}{V_j}(T_{in,ag} - T_{ag}) + \frac{K_T A_T (T_r - T_{ag})}{V \rho_r C_{heat,ag}} \quad (15)$$

Thus, kinetic modeling of alcohol fermentation in continuous fermentation bioreactor is a set of simultaneous equations:

$$\begin{cases} c^*_{O_2,0} = 14.6 - 0.3943 T_r + 0.007714 T_r^2 - 0.0000646 T_r^3 \\ c^*_{O_2} = c^*_{O_2,0} \times 10^{-\sum H_i} \\ r_{O_2} = \mu_{O_2} \dfrac{1}{Y_{O_2}} c_X \dfrac{c_{O_2}}{K_{O_2} + c_{O_2}} \\ \mu_X = A_1 e^{-(E_{a1}/R(T_r+273))} - A_2 e^{-(E_{a2}/R(T_r+273))} \\ \dfrac{dV}{dt} = Fi - Fe \\ \dfrac{dc_X}{dt} = \mu_X c_X \dfrac{c_S}{K_S + c_S} e^{-K_p c_p} - \dfrac{Fe}{V} c_X \\ \dfrac{dc_P}{dt} = \mu_P c_X \dfrac{c_S}{K_{S1} + c_S} e^{-K_{p1} c_p} - \dfrac{Fe}{V} c_P \\ \dfrac{dc_S}{dt} = -\dfrac{1}{R_{SX}} \mu_X c_X \dfrac{c_S}{K_S + c_S} e^{-K_p c_p} + \dfrac{Fi}{V} c_{S,in} - \dfrac{1}{R_{SP}} \mu_P c_X \dfrac{c_S}{K_{S1} + c_S} e^{-K_{p1} c_p} - \dfrac{Fe}{V} c_S \\ \dfrac{dc_{O_2}}{dt} = (k_l a)(c^*_{O_2} - c_{O_2}) - r_{O_2} \\ \dfrac{dT_r}{dt} = \dfrac{Fi}{V}(T_{in} + 273) - \dfrac{Fe}{V}(T_r + 273) + \dfrac{r_{O_2} \Delta H_r}{32 \rho_r C_{heat,r}} + \dfrac{K_T A_T (T_r - T_{ag})}{V \rho_r C_{heat,r}} \\ \dfrac{dT_{ag}}{dt} = \dfrac{F_{ag}}{V_j}(T_{in,ag} - T_{ag}) + \dfrac{K_T A_T (T_r - T_{ag})}{V \rho_r C_{heat,ag}} \end{cases}$$

There are numerous kinetic models for ethanol fermentation. Mathematical models have been used to predict the effect of operating parameters on biomass concentration, substrate utilization rate and ethanol formation rate. The kinetic parameters of the alcohol fermentation were used in this study obtained from the previous experimental data.

Table 1. Parameter values used for simulation

No	Parameter	Nomenclature / Greek symbols	Value/ Unit
1	Pre exponential factors in Arrhenius equation	A_1	9.5×10^8
2	Pre exponential factors in Arrhenius equation	A_2	2.55×10^{33}
3	Heat transfer area	A_T	1, m^2
4	Heat capacity of mass of reaction	$C_{heat,r}$	4.18, $Jg^{-1}K^{-1}$
5	Oxygen concentration in the liquid phase	c_{O_2}	mg/L
6	Equilibrium concentration of oxygen in the liquid phase	$c^*_{O_2}$	mg/L
7	Product (ethanol) concentration	C_P	g/L
8	Substrate (glucose) concentration	C_S	60, g/L
9	Glucose concentration in the feed flow	$C_{S,in}$	g/L
10	Biomass (yeast) concentration	C_X	g/L

11	Apparent activation energy for the growth, respectively, denaturation reaction	E_{a1} E_{a2}	50000 J/mol 220000 J/mol
12	Flow of cooling agent	F_{aq}	L/h
13	Flow of substrate entering the reactor	F_i	L/h
14	Outlet flow from the reactor	F_e	L/h
15	Specific ionic constant of ion i (i = Na, Ca, Mg, Cl, CO3, etc.)	H_i	
16	Ionic strength of ion i (i = Na, Ca, Mg, Cl, CO3, etc.)	I_i	
17	Product of mass-transfer coefficient for oxygen and gas-phase specific area	K_ia	38, h^{-1}
18	Constant of oxygen consumption	K_{02}	8.86 mg/L
19	Constant of growth inhibition by ethanol	K_p	0.139, g/L
20	Constant of fermentation inhibition by ethanol	K_{p1}	0.070, g/L
21	Constant in the substrate term for growth	K_S	1.030, g/L
22	Constant in the substrate term for ethanol production	K_{S1}	1.680, g/L
23	Heat transfer coefficient	K_T	$3.6x10^5$ $Jh^{-1}m^{-2}K^{-1}$
24	Rate of oxygen consumption	r_{O_2}	mg $l^{-1}h^{-1}$
25	Universal gas constant	R	8.31 J $mol^{-1}K^1$
26	Ratio of ethanol produced per glucose consumed for fermentation	R_{SP}	0.435
27	Ratio of cell produced per glucose consumed for growth	R_{SX}	0.067
28	Temperature of cooling agent in the jacket	T_{ag}	15°C
29	Temperature of the substrate flow entering to the reactor	T_{in}	25 °C
30	Temperature in the reactor	T_r	30 °C
31	Volume of the mass of reaction	V	50, L
32	Volume of the jacket	V_j	100, L
33	Yield factor for biomass on oxygen (mg/mg), defined as the amount of oxygen consumed per unit biomass produced	Y_{02}	0.970, mg/mg
34	Reaction heat of fermentation	ΔH_r	518 kJ/mol O_2 đã tiêu thụ
35	Maximum specific oxygen consumption rate	μ_{02}	0.5, L/h
36	Maximum specific fermentation rate	μ_P	1.790, L/h
37	Maximum specific growth rate	μ_X	h^{-1}
38	Density of cooling agent	ρ_{aq}	1000, g/L
39	Density of the mass of reaction	ρ_r	1080

3. RESULTS AND DISCUSSION

The presented dynamic model is simulated by using software tool Simulink as a toolbox package in the Matlab R2016a software.

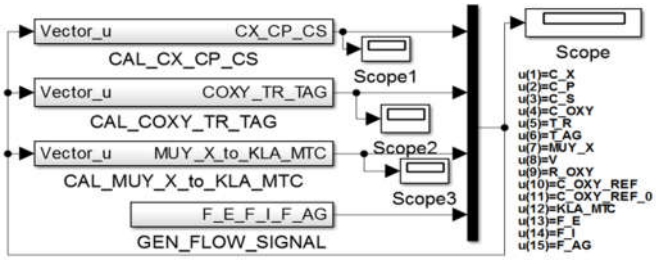

Figure 5. Schematic diagram simulated the overall system

The simulation program was designed according to modularization as presented in Fig. 5. Each of modules contained nonlinear and integral equations to describe a system of equations of state - space for an alcoholic fermentation as the following Fig. 6.

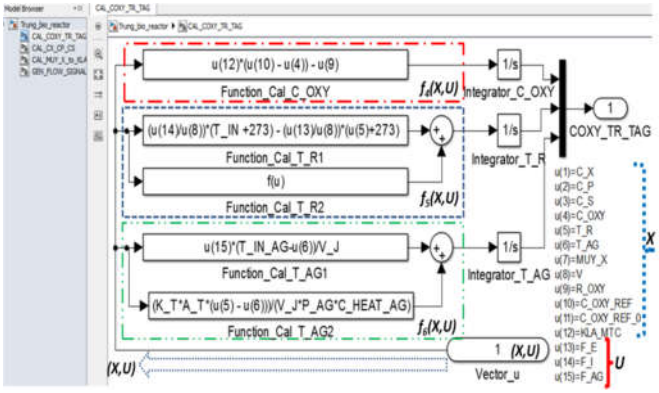

Figure 6. Detailed calculation of CAL_OXY_TR_TAG

The above simulation diagram was used for multiple-cases simulation depending on the kinetic parameters entered via M-file as follows:

- Flow of substrate entering the reactor: $F_i = 51$ (l/h)
- Outlet flow from the reactor: $F_e = 51$ (l/h)
- Glucose concentration in the feed flow: $C_{S,in} = 60$ (g/l)
- Temperature of cooling agent in the jacket: $T_{ag} = 15$°C.
- Temperature of the substrate flow entering to the reactor: $T_{in} = 25$°C
- Simulation - time: t = 60 (h)

Simulation results obtained as follows:

- Simulation results using Runge-Kutta (4,5)[6]
- The comparison of the results between ode45 and ode23 solvers.

In the Fig. 7 showed the result of fermentation process. In the first 1 hour, it's the lag phase for yeast acclimate for the environment so the reactor temperature decreased by cooler agent. At the log phase (about 10 hours after lag phase) where cells are rapidly growing and dividing that's increase temperature in the reactor and then the reactor temperature was controlled by the cooler agent.

The two graphs (Fig. 8) shown that using Runge-Kutta (4,5) method(ode45) with higher convergence than Runge-Kutta (2,3) method(ode23). A smaller calculation step given more accurate results. The simulation results are closely relevant with data obtained from the previous

experimental. This simulation allows engineers to perform different analysis in order to select the best parameter for operating fermentation process. The application of this simulation method will open the prospect of simulating multiple fermentation processes in food technology and biotechnology.

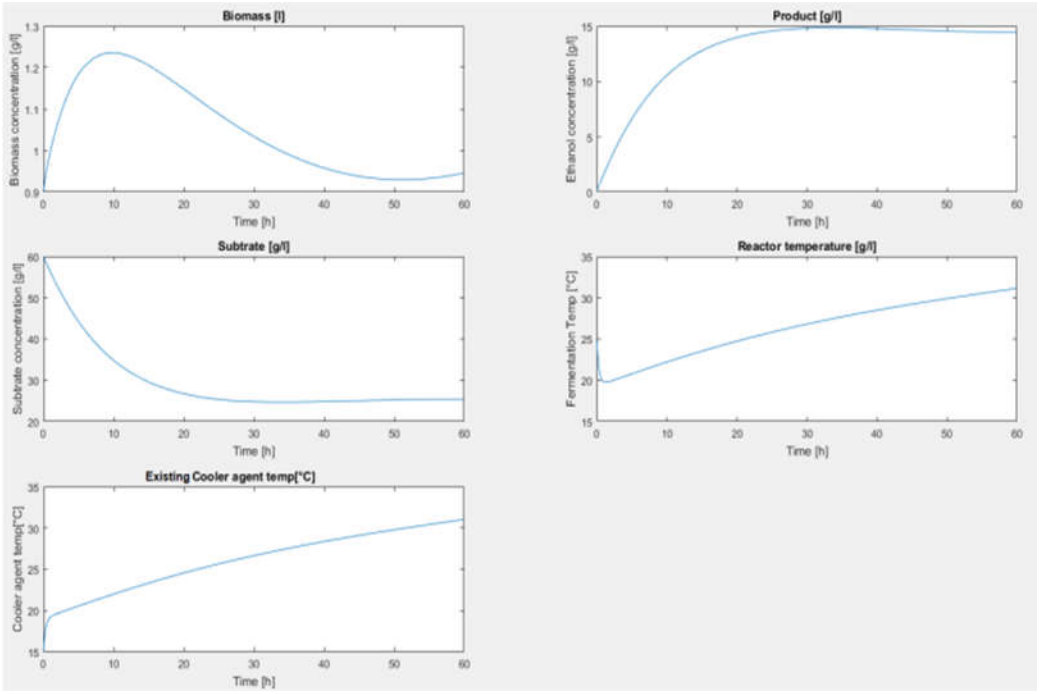

Figure 7. Simulation results using Runge-Kutta

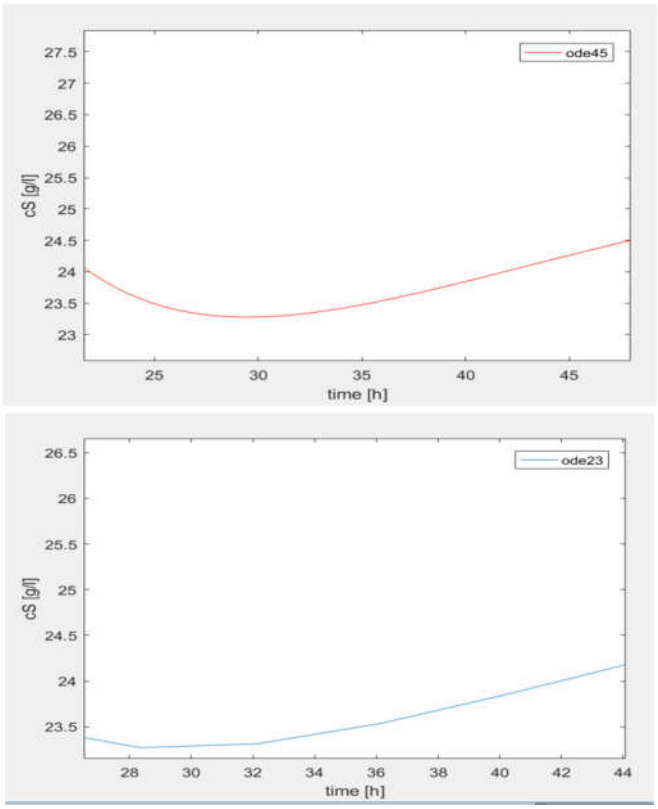

Figure 8. The comparison of the results between ode45 and ode23 solvers

4. CONCLUSIONS

In this work, we have simulated the modelling of alcohol fermentation process by Simulink® which a tool of Matlab®. Accordingly, using mathematical models and simulation tools have predicted the result and reducing time and labor experimental works. We showed the using Runge-Kutta (4,5) algorithm (ode45) was better result than Runge-Kutta (2,3) algorithm (ode23). Choosing calculation method is also important that effect to conclusions.

REFERENCES

[1]. Cheng Y., T.W. Karjala, D.M. Himmelblau, 1995. *Identification of Nonlinear Dynamic Processes with Unknown and Variable Dead Time Using an Internal Recurrent Neural Network.* Industrial & Engineering Chemistry Research, 34(5): p. 1735-1742.

[2]. Roels J.A., 1982.*Mathematical models and the design of biochemical reactors.* Journal of Chemical Technology and Biotechnology, 32(1): p. 59-72.

[3]. Aiba S., M. Shoda, M. Nagatani, 2000. *Kinetics of product inhibition in alcohol fermentation.* Reprinted from Biotechnology and Bioengineering, Vol. X, Issue 6, Pages 845-864 (1968). Biotechnol Bioeng, 67(6): p. 671-90.

[4]. Sevella B., 1992. *Bioengeneering Operations.* Technical University of Budapest, Tankonykiado, Budapest.

[5]. Godia F., C. Casas, C. Sola, 1988. *Batch alcoholic fermentation modelling by simultaneous integration of growth and fermentation equations.* Journal of Chemical Technology & Biotechnology, 41(2): p. 155-165.

[6]. Dormand J.R., P.J. Prince, 1980. *A family of embedded Runge-Kutta formulae.* Journal of Computational and Applied Mathematics, 6(1): p. 19-26.

THÔNG TIN TÁC GIẢ

Trần Văn Tài, Nguyễn Trường Giang, Nguyễn Đức Trung

Viện Công nghệ sinh học và Công nghệ thực phẩm,
Trường Đại học Bách khoa Hà Nội