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Proceeding

The 2nd International Conference of the Indonesian Chemical Society 2013

ICICS 2013

Research in Chemistry for Better Quality of Environmental

Universitas Islam Indonesia, Yogyakarta, Indonesia
October, 22 - 23th 2013

Abdul Kahar Muzakkir, Conference Hall
Universitas Islam Indonesia (UII), Yogyakarta.
Kampus Terpadu, Jl. Kaliurang KM 14,5 Sleman, Yogyakarta.

Preface

The international conference is an annual conference of the Indonesian Chemical Society (Himpunan Kimia Indonesia, HKI). In the year 2013, the mandate of the organizing committee was given to the HKI Yogyakarta branch and also supported by Department of Chemistry of Universitas Negeri Yogyakarta (UNY), Department of Chemistry of Universitas Gadjah Mada (UGM), Department of Chemistry of Universitas Islam Negeri Sunan Kalijaga (UIN Suka), National Nuclear Energy Agency (BATAN Yogyakarta), and Volcano Investigation and Technological Development Center (BPPTK Yogyakarta). For the year 2013, ICICS 2013 is hosted by Department of Chemistry, Faculty of Mathematics and Natural Sciences, Islamic University of Indonesia, Yogyakarta from October 22 – 23, 2013. This conference was also prepared to celebrate 70th anniversary of Universitas Islam Indonesia.

The Sicentific Programme of ICICS2013 comprises the following:

1. Invited Speaker 11 papers
2. A total 256 paper for parallels sessions
    a. Organic Chemistry 32 papers
    b. Inorganic Chemistry 43 papers
    c. Physical Chemistry 37 papers
    d. Analytical Chemistry 68 papers
    e. Education Chemistry 23 papers
    f. Biochemistry 43 papers

The breakdown of the presentation is as follows:

Session	Oral	Poster	Total
Invited Speaker	11	0	11
Organic Chemistry	25	7	32
Inorganic Chemistry	38	5	43
Physical Chemistry	31	6	37
Analytical Chemistry	61	7	68
Education Chemistry	22	1	23
Biochemistry	34	8	43
Total	**222**	**34**	**256**

Yogyakarta, 25th November 2013

Editors

Welcoming Address by The Organizing Committee

Assalamu'alaikum Wr. Wb.

Honorable Rector of Universitas Islam Indonesia
The distinguished invited speakers, and
All participants of the ICICS 2013

Welcome you at the 2nd International Conference of the Indonesia Chemical Society 2013 (ICICS 2013) this morning here at the Auditorium Kahar Muzakkir Universitas Islam Indonesia, Yogyakarta. The international conference is an annual conference of the Indonesian Chemical Society (Himpunan Kimia Indonesia, HKI). In the year 2013, the mandate of the organizing committee was given to the HKI Yogyakarta branch and also supported by Department of Chemistry of Universitas Negeri Yogyakarta (UNY), Department of Chemistry of Universitas Gadjah Mada (UGM), Department of Chemistry of Universitas Islam Negeri Sunan Kalijaga (UIN Suka), National Nuclear Energy Agency (BATAN Yogyakarta), and Balai Penyelidikan dan Pengembangan Kegunungapian (BPPTK Yogyakarta). For the year 2013, the honor of hosting ICICS 2013 has been given to the Department of Chemistry, Faculty of Mathematics and Natural Sciences, Universitas Islam Indonesia, Yogyakarta. This conference was also prepared to celebrate 70th anniversary of Universitas Islam Indonesia.

The conference comprises both oral and poster presentation in English and Indonesian with optional post conference publication of full papers in English in the Procedia Chemistry (Elsevier, ISSN: 1876-6196) and Proceeding Conference for Indonesian language. There are 211 papers presented orally and 34 papers presented by poster covering wide-variety subjects of chemistry. We invited 6 Indonesian invited speakers, 2 Japan invited speakers, 1 Australian invited speakers, 1 Saudi Arabia invited speakers, and 1 Malaysian Invited speakers.

We hope you will enjoy a pleasant and valuable seminar at Universitas Islam Indonesia

Wassalamu'alaikum Wr. Wb.

Riyanto, Ph.D.

Chairman

Opening Speech from the Rector of Universitas Islam Indonesia

Assalamu'alaikum Wr. Wb
The distinguished invited speakers, and
All participants of the ICICS 2013

Firstly, I would like to express my great appreciation to the Department of Chemistry UII as one of the organizers of the program The 2nd International Conference of the Indonesian Chemical Society 2013 (ICICS 2013) with the theme "Research in Chemistry for Better Quality of Environmental". I am proud that this interesting event is being organized and held in Yogyakarta.
As the biggest and the oldest private university in Yogyakarta, University Islam Indonesia is committed to the excellence in research and teaching. Recently, we are preparing UII as one of the world class universities.
Knowing that committee has selected outstanding speakers from various prestigious institutions. I believe that all of the participants will enjoy the discussion of issue covered by the topic of this seminar. Scientist have shown that the environment's condition is increasingly critical, and human industrial activities are largely to blame. In fact that environmental damage is a crisis we caused together, therefore, a responsibility we all share together. We are deeply concerned with the issues and opportunities in the internationalization of sciences for better life, sciences have to make better quality of environmental.
Finally, I would once again like to thank the organizer for organizing this event, and to thank all the participants attending this ICICS 2013 event as well as delivering their scientific presentations. I do really hope that you can enjoy this seminar and have excellent stay in Yogyakarta.

Wassalamu'alaikum Wr. Wb

Prof. Dr. Edy Suandi Hamid, M.Ec.
Rector of Universitas Islam Indonesia

Remarks by the Chairman of the Indonesian Chemical Society (Himpunan Kimia Indonesia, HKI)

Indonesian Chemical Society (Himpunan Kimia Indonesia, HKI) is an independent, nonprofit organization founded in February 1962 to facilitate communication among Indonesian chemists and other professionals from chemistry related fields, and to promote the advancement of science, education, and application of chemistry to support the better life of mankind. HKI organize activities to enhance communication and collaboration among chemists in various institutions in Indonesia, to disseminate new knowledge and research results in chemistry and related fields, to improve the knowledge and skills of chemists working in schools, universities, industries, research institutes, and other sectors, to nurture a scientific temper on school children to ensure strong capabilities of future chemists that are needed for humankind, and other activities that support its missions. HKI holds various academic conferences, publishes several journals, supports the development of scientific information systems in Indonesian; organize training for chemists in various sectors, etc.

The 2013 International Conference of the Indonesian Chemical Society will be the 2nd event in the ICICS conference series, started in 2012, that brings together individuals involved in chemistry-related fields (chemistry, pharmacy, environmental science, chemical engineering, molecular biology, material science, education chemistry, etc.) or institution in chemistry-related sectors. The First International Conference of the Indonesian Chemical Society 2012 is organized by East Java Branch of HKI in collaboration with chemistry departments at several universities in East Java: ITS, UB, UIN Maliki, UM, UMC, Unair, Unej, and Unesa.

ICICS 2013 will be organized by the Indonesian Chemical Society Yogyakarta branch. The international conference was supported by the Indonesian Chemical Society (Himpunan Kimia Indonesia, HKI), Department of Chemistry of Universitas Negeri Yogyakarta (UNY), Department of Chemistry of Universitas Gadjah Mada (UGM) and Department of Chemistry of Universitas Islam Negeri Sunan Kalijaga (UIN Sunan Kalijaga). For the year 2013, the honor of hosting ICICS-2013 has been given to the Department of Chemistry, Faculty of Mathematics and Natural Sciences, Universitas Islam Indonesia (UII), Yogyakarta, Indonesia.

Congratulations to the ICICS 2013 committee for this conference.

Dr. Muhamad Abdulkadir Martoprawiro
Chairman of the Indonesian Chemical Society

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Bioprocess System Identification of Continuous Fermentation

Rudy Agustriyanto*, Akbarningrum Fatmawati

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Abstracts

Bioprocess models are very important in bioprocess control. A bioprocess model refers to the mathematical representation of the biophysical and biochemical phenomena taking place in the process. Such model can help to understand the plant behavior and can assist in avoiding excessive experimentation. In bioprocess control system design, bioprocess model is used as a tool in many stages such as: control structure selection, stability analysis, and tuning controller parameters. This paper will present bioprocess system identification of continuous fermentation for gluconic acid production. In this study, the input and output data was generated from first principle dynamic bioprocess model using *Contois* kinetic model and mass balances. The data was then analyzed using *System Identification Toolbox* in Matlab. The final results obtained are in the form of Laplace-transfer functions which will be very useful for the above mentioned purposes.

Introduction

The different applications of process models and the different modeling goals have lead to many different model classifications as shown in Figure 1. There are numerous books and articles on theoretical process modeling but they all have similar approach which is outlined in Figure 2 (Lee et al., 1998). This shows that modeling involves some clearly defined steps and incorporates some iteration in the process. This comes from program verification and model validation or refinement.

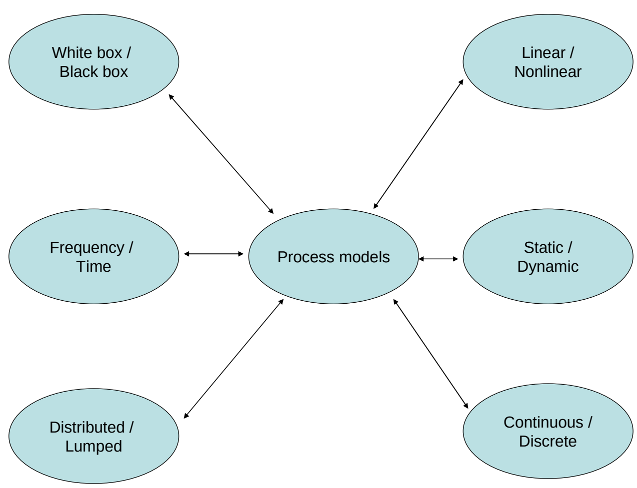

Figure 1 Model classifications

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Several notable previous studies regarding gluconic acid production through fermentation include Liu et al (2003) who proposed mathematical model for gluconic aid fermentation by *Aspergillus niger* and reported that the model could provide reasonable description of the processes. Znad et al (2004) investigated the production of gluconic acid from glucose for growth and non-growth conditions in batch reactor. Klein et al (2002) studied the mass transfer in an airlift bioreactor for the biotransformation of glucose to gluconic acid by *Aspergillus niger*.

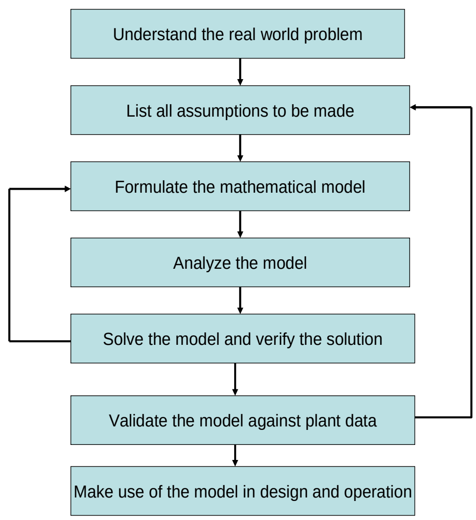

Figure 2.

Model of Continuous Fermentation for Gluconic Acid Production

Figure 3 shows the continuous fermentation system used in this study. In the system, feed with glucose concentration S_i enters the fermenter at constant volumetric flowrate of Q. Gluconic acid will appear in product stream with concentration P_o as a result of glucose fermentation of the cell (*Aspergillus niger*). The concentrations of the cell in the inlet and outlet of the fermenter are denotes as X_i and X_o respectively and the remaining glucose concentration at the fermenter outlet is S_o. At certain volumetric flowrate, the gluconic acid product concentration will depend on the volume of the fermenter. The condition of the fermenter shown in Figure 1 was to be kept constant at pH of 5.5 and the ratio of aeration rate to the fermenter volume of 1.

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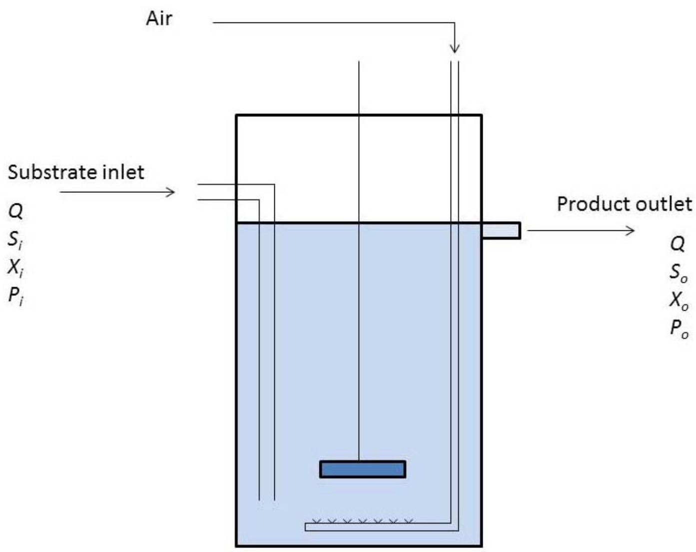

Figure 3. Schematic of continuous fermentation system

The cell growth model used in this research is *Contois* equation which can be written as follows:

$$\mu = \mu_m \frac{S}{K_S^{'} X + S} \tag{1}$$

Where:

μ = specific growth rate, 1/h

X = cell concentration, g/L

S = substrate concentration, g/L

μ_m = maximum specific growth rate, 1/h

$K_S^{'}$ = *Contois* saturation constant

The *Contois* model describes cell inhibition on the growth which is suitable for fermentation with high cell density.

In batch fermentation, the mass balance of the cell, substrate and product can be written as follows:

$$\frac{dX}{dt} = r_X = \mu X \tag{2}$$

$$\frac{dS}{dt} = r_S = \frac{1}{Y_{X/S}} \frac{dX}{dt} - \frac{1}{Y_{P/S}} \frac{dP}{dt} - m_S X \tag{3}$$

$$\frac{dP}{dt} = r_P = \alpha \frac{dX}{dt} + \beta X \tag{4}$$

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Where:

$Y_{X/S}$ = yield coefficient for cell on substrate

$Y_{P/S}$ = yield coefficient for product on substrate

m_S = maintenance energy coefficient, 1/h

P = product concentration, g/L

α = growth associated product formation constant

β = non-growth associated product formation constant, 1/h

t = time, h

r_X = cell growth rate, g/L.h

r_S = substrate consumption rate, g/L.h

r_P = product growth rate, g/L.h

Continuous fermentation as shown in Figure 3 can be modeled based on the mass balance equation of cell, substrate and product (Fatmawati and Agustriyanto, 2010). The models are as follows:

$$\frac{dX}{dt}V = QX_i + \frac{\mu_m SX}{K_S^{'}X + S}V - QX \tag{5}$$

$$\frac{dS}{dt}V = QS_i - \left(\frac{1}{Y_{X/S}}\frac{\mu_m SX}{K_S^{'}X + S} + m_S X + \frac{1}{Y_{P/S}}\left(\alpha\frac{\mu_m SX}{K_S^{'}X + S} + \beta X\right)\right)V - QS_o \tag{6}$$

$$\frac{dP}{dt}V = QP_i + \left(\alpha\frac{\mu_m SX}{K_S^{'}X + S} + \beta X\right)V - QP \tag{7}$$

The *Contois* kinetic parameters for gluconic acid production have been studied previously (Fatmawati and Agustriyanto, 2010) and are shown in Table 1 along with steady state operating condition of continuous fermentation system.

Table 1. Steady state operating conditions and Contois kinetic parameters

Operating Parameters	Values	
Steady State Values:		
Hydraulic retention time, *R=V/Q*	24	h
Inlet cell concentration, *Xss*	0	
Inlet substrate concentration, S_{SS}	150	g/L
Inlet product concentration, P_{SS}	0	
Outlet cell concentration, *X*	9.3843	g/L
Outlet substrate concentration, *S*	31. 8372	g/L
Outlet product concentration, *P*	0.0863	g/L
Kinetic Parameters:		
Maximum specific growth rate, μ_m	1.2698	h^{-1}
Contois saturation constant, $K_S^{'}$	99.9963	
Yield coefficient of cell, $Y_{X/S}$	0.1006	
Yield coefficient of product, $Y_{P/S}$	0.5000	
Maintenance coefficient, m_S	0.1097	h^{-1}
Growth associated product constant, α	0.0068	
Non growth associated product constant, β	0.0001	h^{-1}

Method

Although a first principle models are available for the continuous fermentation, here linear models are identified from the simulated bioprocess operation data using the nonlinear simulator. This is because in practical applications, bioprocess models are generally not available and have to be identified from bioprocess operation data. Step tests were performed for input variables. The complete transfer function expected is in the form (Ljung, 1997):

$$y = G.u \tag{8}$$

Where:

$$y = \begin{bmatrix} X \\ S \\ P \end{bmatrix} \tag{9}$$

$$G = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix} \tag{10}$$

$$u = \begin{bmatrix} X_i \\ S_i \\ P_i \end{bmatrix} \tag{11}$$

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Results and Discussion

Individual step test were performed for all input variables of its nominal steady state at t = 5 h. Process responses are sampled every 10 minutes and collected for 24 h simulation time from simulation based on the non-linear model provided in the form of differential equations. The complete identified transfer functions is as follows:

$$G = \begin{bmatrix} \frac{0.83941}{2.9988s+1} & \frac{0.06313}{3.66s+1}e^{-0.60015s} & 0 \\ \frac{-0.6495}{3.6345s+1}e^{-0.59496s} & \frac{0.21932}{0.57501s+1} & 0 \\ \frac{0.0010058}{5.4411s+1}e^{-0.59553s} & \frac{0.000584}{4.7609s+1}e^{-0.6485s} & \frac{0.99689}{3.7515s+1} \end{bmatrix} \quad (12)$$

Plots of actual responses and the simulated values using the identified models are shown in Figures 4 to 6. It can be seen from Figures 4 to 6 that the models are satisfactory in that the model simulated values (long range predictions) are very close to the actual process values.

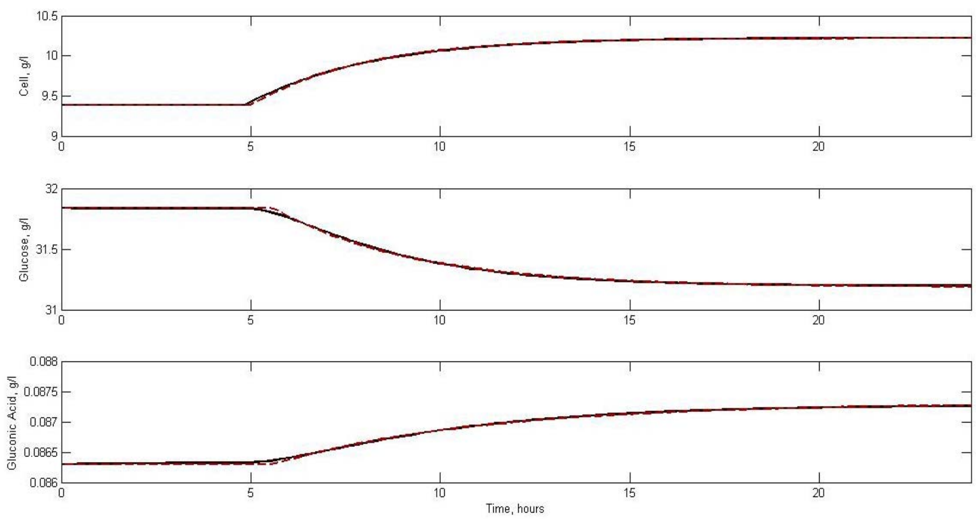

Figure 4. Actual process outputs and the simulated values from the identified model for a unit step up of inlet cell concentration at t=5 hours(___ actual values, ---- predicted values)

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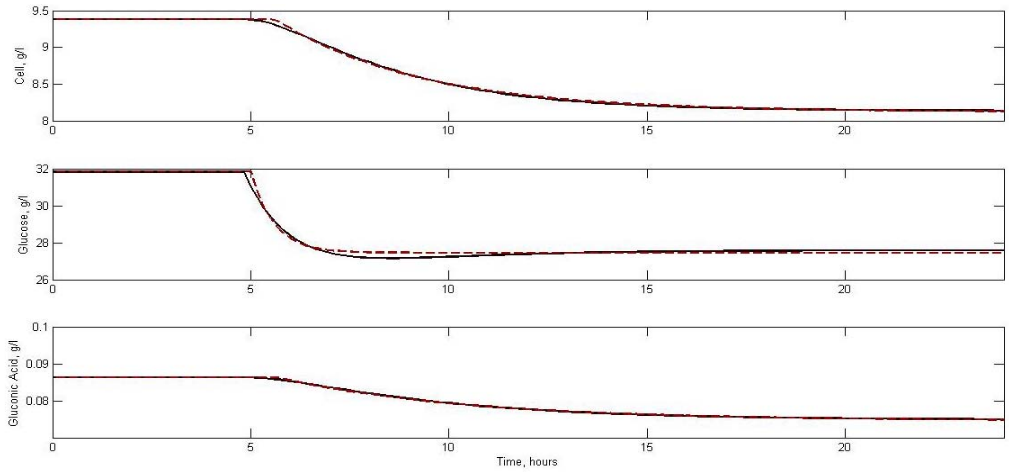

Figure 5. Actual process outputs and the simulated values from the identified model for a 0.01 step up of inlet gluconic acid concentration at t=5 hours (___ actual values, ---- predicted values)

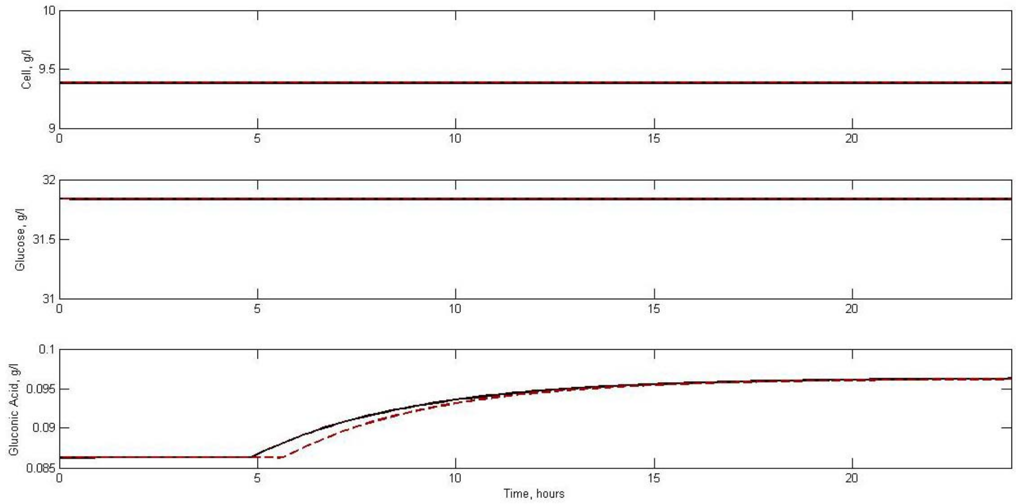

Figure 6. Actual process outputs and the simulated values from the identified model for a unit step up of inlet product concentration at t=5 hours(___ actual values, ---- predicted values)

Conclusions

Bioprocess system identification has been done for continuous fermentation of gluconic acid production using *Aspergillus niger*.The resulting models are in the form of Laplace transfer functions and able to give satisfactory prediction.

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