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Proceedings of the 3rd International Conference on Computation for Science and Technology

The 3rd International Conference on Computation for Science and Technology (ICCST-3) is an international conference dedicated to promoting advances in computational methods for science and engineering. Building on the previous successful meetings, ICCST-1 (2010) in Chiang Mai-Thailand and ICCST-2 (2012) in Nigde-Turkey, this conference program aims to

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To facilitate researchers in Asia-Pacific in dissemination of their recent findings in computation and its application in science and technology. Institut Teknologi Bandung, Indonesia;Chiang Mai University, Thailand; Islamic Azad University, Iran;University Sains, Malaysia; Universitas Udayana Indonesia; Ankara University, Turkey; Kastamonu University, Turkey; Himpunan Kimia Indonesia (HKI); and Indonesian Society of Medicinal Chemistry will co-organize on The 3rd International Conference on Computation for Science and Technology which will be held in Aston Denpasar Hotel and Convention Centre, Bali, September 23rd-25th, 2014.

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Proceedings of the 3rd International Conference on Computation for Science and Technology

The 3rd International Conference on Computation for Science and Technology (ICCST-3) has been held in Bali, Indonesia, on 23-25 September 2014. ICCST-3 is an international conference dedicated to promoting advances in computational methods for science and engineering. Building on the previous successful meetings, ICCST-1 (2010) in Chiang Mai-Thailand and

ICCST-2 (2012) in Nigde-Turkey, this conference program aims to further foster and stimulate international scientific exchange and collaboration. ICCST-3 was co-organized by Bandung Institute of Technology, Indonesia; Chiang Mai University, Thailand; Islamic Azad University, Iran; University Sains, Malaysia; Universitas Udayana, Indonesia; Ankara University, Turkey; Kastamonu University, Turkey, and supported by Indonesian Chemical Society and Indonesian Society of Medicinal Chemistry. The scientific program included plenary and invited lectures to highlight some of the major developments in computational methods for science and engineering, as well as oral session and poster session in disseminating new finding in each field.

Computational method has been applied in sciences, engineering and other related disciplines, such as computational chemistry, computational physics, computational biology, computational mathematics, computational mechanics for solids and structures, computational fluid dynamics, computational heat transfer, computational inverse problem, computational meso/micro/nano mechanics, computational penetration mechanics, molecular and quantum methods, information technology, etc. By computational method, many monumental breakthrough have been achieved in science and engineering for promoting better life.

In collaboration with Atlantis Press, selected papers presented in the conference have been reviewed and published in the proceedings. Finally, 35 papers have been accepted to be published in these proceeding. The papers are coming from the field of computational chemistry, computer-aided drug design, computational mathematics, and computational physics.

We wish thank to invited speakers and participants for sharing and active contribution in the conference. We also greatly thank to all co-organizers and sponsors for supporting the conference. We also thank to advisory board, member of scientific committee and organizing committee in running the ICCST-3 and making the conference be success and fruitful meeting. Finally, we express our deepest thank to the reviewers, readers as well as technical assistant for their professional support in managing and processing papers for proceeding.

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Molecular Docking and Molecular Dynamics Simulation of the Interaction of Cationic Imidazolium Porphyrin-Anthraquinone and Hsp90

Muhammad Arba, Rahmana Emran Kartasasmita, Daryono H. Tjahjono

Hsp90 is involved in the progressiveness of cancer cell through the activation of oncogenic client proteins, including Her2/ErbB2, Akt, Raf-1, and hTERT. Thus, targeting Hsp90 is considered as one of promising strategy in anti-cancer drug development. In the search of new potential Hsp90 inhibitors,...

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In Silico Study of The Component of Eleutherine americana MERR. on Human Estrogen Reseptor Alpha as Potential Anti-Breast Cancer

Tasia Amelia, Dina Pratiwi, Romsiah, Daryono H. Tjahjono

Eleutherine americana (Indonesian: “bawang dayak”) has been used traditionally to treat breast cancer by Borneo people. Its compounds contains eleutherine, eleutherinone,

eleutherol, isoeleutherine, eleutherinol, dihydroeleutherinol, hongconin, and 6,8-dihydroxy-3,4-dimethoxy-1-methyl-anthraquinone-2-carboxylic...

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Pyrazolylporphyrin Derivatives as New Potential Ligand for Melanoma Cancer Radiopharmaceutical Kit: In Silico Study

Fransiska Kurniawan, Rahmana Emran Kartasasmita, Daryono H. Tjahjono

Melanoma is the most lethal skin cancer, and it is related to Fibroblast Growth Factor 2 (FGF2) which is important for survival and proliferation of melanocytes. Diagnosis and therapy of melanoma cancer can be performed applying radiopharmaceutical with appropriate ligand. The aim of this research was...

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Complexes Formation of Porphyrin Derivatives with Lead: Preliminary Computational Study of Porphyrin as Analytical Reagent

Rimadani Pratiwi, Slamet I. Surantaatmadja, Daryono H. Tjahjono

Interaction of three cationic porphyrins: meso-tetrakis (N-methylpyridinium-4-yl) porphyrin (H2TMPyP), meso-tetrakis (1,3-dimethylimidazolium-2-yl)porphyrin (H2TDMImP), and meso-tetrakis(1,2-dimethylpyrazolium-4-yl) porphyrin (H2TDMPzP) with lead have been performanced computationally using DFT method....

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Interactions of Porphyrin-Acridine Hybrids to DNA Duplexes and Quadruplex: In Silico Study

Hubbi Nashrullah Muhammad, Sophi Damayanti, Daryono H. Tjahjono

The binding modes of cationic porphyrin hybrids to DNA has been studied in a previous study. In the present research, cationic porphyrin-acridine hybrids bearing meso-substituted pyridine, imidazole, and pyrazole rings were investigated for their interaction with DNA. AutoDock Vina was used to dock 11...

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Toxicity Prediction of meso-5,15-di[3,4-bis(carboxymethylenoxy)phenyl] porphyrin and meso-5,15-di[3,4-bis(carboxymethylenoxy)phenyl],10,20-

diphenyl porphyrin

Fauzan Zein Muttaqin, Slamet I. Surantaatmadja, Abdul Mutalib, Daryono H. Tjahjono

Porphyrin and its derivatives are widely investigated for cancer therapy because of their high selectivity to cancer cells. By labeling gamma and beta emitting-radionuclides to a porphyrin which selectively binds to the cancer tissue will produce a safe and potential radiopharmaceutical. The present...

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Absorption, Distribution and Toxicity Prediction of Curculigoside A and its Derivatives

Nursamsiar, Slamet I. Surantaatmadja, Daryono H. Tjahjono

Curculigoside A is a major bioactive phenolic glycoside of the medicinal plant of Curculigo orchioides. The present study was intended to obtain detail information of the pharmacokinetic properties including oral absorption, distribution, metabolism and toxicity of curculigoside A and its derivatives...

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In Silico Study of Andrographolide as Protease Inhibitors for Antimalarial Drug Discovery

Sandra Megantara, Jutti Levita, Slamet I. Surantaatmadja

Malaria parasite encodes several homologues of aspartic proteases such as plasmepsin I, II and IV which are responsible for degradation of host erythrocyte hemoglobin inside the vacuole of parasite food. Hence plasmepsins are novel targets for antimalarial drug discovery. Previous study concluded that...

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Nursamsiar, Lina Nurfadhila, Iman S. Pratama, Aiyi Asnawi, Slamet I. Surantaatmadja

Chemokine receptor CCR5, a G protein-coupled receptor (GPCR), has been shown as a viable target in drug discovery due to its involvement in HIV entry and cancer. In HIV pathogenesis, CCR5 acts as an essential co-receptor for HIV invasion into host cells; whereas in cancer, it provides a pro-inflammatory...

Acetylation of Asiatic Acid and Its Hepatotoxicity Prediction

Ida Musfiroh, Ita Puspitasari, Ahmad Muhtadi, Rahmana E. Kartasasmita, Slamet I. Surantaatmadja

Asiatic acid (AA) is one of the triterpenoids isolated from pegagan (Centella asiatica (L.) Urb.), which has the antiinflammatory activity. The present studies were aimed to synthesize triacetyl asiatic acid (2,3,23-triacetooxy-12-ene asiatic acid) and to predict its hepatotoxicity properties. Acetylation...

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Prediction of Hazard Identification and Characterization of Several Compounds used as Food Additives Applying In Silico Methods

Iltizam Nasrullah, Rahmana Emran Kartasasmita, Sophi Damayanti

In frame of risk analysis, hazard identification and characterization are parts of risk assessment that should be performed to assure the safety aspect of a substance that will be

used as food additive. According to WHO guidance, the two steps can be performed experimentally, based on epidemiological...

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Discovering Inhibitors of Tyrosinase Enzyme from Zingiberaceae for Depigmentation Agents

Karina Muthia, Fride Rindu Alami, Nyi Mekar Saptarini, Jutti Levita

Tyrosinase enzyme, which has two copper ions in its catalytic site, involved in skin pigmentation by catalyzing three oxidation reactions on melanogenesis, that are conversion of L-tirosine to L-DOPA, L-DOPA to dopaquinone, and 5,6-dihydroxyindole to 5,6-indolequinone. An inhibition of melanogenesis...

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Computational Design of Dengue Type-2 NS2B/NS3 Protease Inhibitor: 2D/3D QSAR of Quinoline and Its Molecular Docking

Maywan Hariono, Ezatul E. Kamarulzaman, Habibah Wahab

The reemergence of dengue outbreak demands an effective and efficient treatment especially for antiviral agent since neither vaccine nor drug is available to overcome this disease. This study designed the new model for Dengue Type-2 (DENV2) NS2B/NS3 protease inhibitor from quinoline scaffold by combining...

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Docking of Dengue NS2B-NS3 Protease with Murraya koenigii

Kai Sing Yong, Sy Bing Choi, Habibah Wahab

Dengue disease has been reported for more than 100 million cases every year distressing tropical and subtropical countries. Dengue virus carries a positive single strand RNA, belongs to Flaviviridae family consist of four serotypes give rise to undifferentiated fever, dengue fever (DF), dengue hemorrhagic...

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Molecular Dynamics Simulation on Designed Antibodies of HIV-1 Capsid Protein (p24)

Hana Atiqah Abdul Karim, Chatchai Tayapiwatana, Piyarat Nimmanpipug, Sharifuddin M. Zain, Noorsaadah Abdul Rahman, Vannajan Sanghiran Lee

Computational approaches have been used by the molecular biologists all around the world as a vital tool in developing and improving the functional and binding properties of proteins, particularly antibody-antigen (Ab-Ag) complexes. Based on a previous work, it has been identified that several residues...

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Computer-aided Structure-based Design of 3,3'-Diallyl-[1,1'-biphenyl]- 4,4'-diol Analogs of Eugenol as Potential Ligands for Estrogen Receptor Alpha

Enade Perdana Istyastono, Yulia Anita, Andini Sundowo

The SBVS protocols to identify ligands for estrogen receptor alpha (ER) were retrospectively validated and could serve as a virtual tool to screen potential ER ligands. Subsequently, prospective virtual screen campaigns on eugenol analogs and their dimers were performed and have discovered 3,3'-diallyl-[1,1'-biphenyl]-4,4'-diol...

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Computational Alanine Scanning Mutagenesis: Characterizing the hotspots of ILK-Ankyrin Repeat and PINCH1 Complex

Vertika Gautam, Nadia Hanim Sabri, Wei Lim Chong, Sharifuddin M. Zain, Noorsaadah Abd. Rahman, Vannajan Sanghiran Lee, Anand Gaurav

From the last two decades, computational alanine scanning mutagenesis (cASM) have been successively applied to a variety of protein complexes to study the energetics and structural characteristics of hot spot residues at protein interface. The cASM combines a continuum approach to model solvent interactions...

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Molecular Docking Studies of Flavonoids of Noni Fruit (Morinda citrifolia L.) to Peroxisome Proliferator-Activated Receptor-Gamma (PPAR)

Fikry Awaluddin, Andrianopsyah Mas Jaya Putra, Supandi Supandi

Diabetes is a chronic disease that occurs either when the pancreas does not produce enough insulin or when the body cannot effectively use the produced insulin. Morinda citrifolia has been widely used as herbal medicine to prevent and to treat diabetes as well as health supplements. It contains flavonoids...

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Exploration of Residue Binding Energy of Potential Ankyrin for Dengue Virus II from MD Simulations

Wei Lim Chong, Sharifuddin M. Zain, Noorsaadah Abd. Rahman, Rozana Othman, Shatrah Binti Othman, Piyarat Nimmanpipug, Chatchai Tayapiwatana, Vannajan Sanghiran Lee

Computational approach was employed to evaluate the binding activity of potential ankyrin and domain III of the envelope protein of dengue virus II. Ankyrin serves as an alternative to antibody due to several advantages. Both the ankyrin and domain III were docked using Z-dock protocol in Discovery Studio...

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Binding Models of Polyphenols to Cytochrome P450 2C9: A Molecular Docking Study

Siripat Chaichit, Darunee Hongwiset, Supat Jiranusornkul

Polyphenols are widely presented in plants and dietary supplements. The beneficial effects of these compounds have been demonstrated, including the prevention of cardiovascular

diseases, osteoporosis, neurogenerative diseases and diabetes. From previous studies, polyphenols showed the inhibitory effect...

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Virtual Screening of 2-hydroxy-1,4-naphthoquinone Derivatives as Antimitotic Agent using Molegro Virtual Docker on Polo Like Kinase 1

Susi Kusumaningrum, Soleh Kosela, Wahono Sumaryono, Emil Budianto, Alfan Danny Arbianto

Naphthoquinone is one of secondary metabolites that are widespread in nature and found in large amounts [1]. Naphthoquinones are clinically important antitumor drugs containing a quinone moiety, such as anthracyclines, mitoxantrones and saintopin, show excellent anticancer activity [2]. In the previouse...

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QSAR Study of Quinazoline Derivatives as Inhibitor of Epidermal Growth Factor Receptor-Tyrosine Kinase (EGFR-TK)

La Ode Aman, Widisusanti Abdulkadir, Julitha Geybie Rembet, Daryono H. Tjahjono

Nowadays a lot of new active substances as anticancer cervix agents have been developed. One of the protein targets in discovery of anticancer cervix drugs is Epidermal Growth Factor Receptor-Tyrosine Kinase (EGFR-TK). In this present research the Quantitative Structure and Activity Relationship (QSAR)...

Cembranoid Diterpenes as Antitumor: Molecular Docking Study to Several Protein Receptor Targets

Muhammad S. Zubair, Syariful Anam, Khalid O. Al-Footy, Ahmed Abdel-Lateef, Walied M. Alarif

A molecular docking analysis has been carried out on several cytotoxic cembaranoid type diterpenes that have been isolated from soft coral Sarcophyton glaucum i.e sarcophytolol, sarcophytolide B, sarcophytolide C, sarcophine, deoxosarcophine, and cembrene C. All the compounds were investigated using...

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Numerical Analysis on the Stability Behavior of a Dynamical System on the Deposit and Loan of a Bank

Novriana Sumarti, H. Fansuri

A dynamical system is one of sophisticated techniques using mathematical equations that can determine the observed state for all future times based on the current state. It will also show small changes in the state of the system create either small or big changes in the future depending on the model....

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Implementation of Finite Field Arithmetic Operations for Polynomial and Normal Basis Representations

Mirza Maulana, Wenny Franciska Senjaya, Budi Rahardjo, Intan Muchtadi-Alamsyah, Marisa W. Paryasto

Elliptic Curve Cryptography is generally are implemented over prime fields or binary fields. Arithmetic in binary elds can be classified according to the basis representation being used. Two of the most common basis used in binary elds are polynomial basis and normal basis. The optimal normal basis is...

Reducing Computational Complexity of Network Analysis using Graph Compression Method for Brand Awareness Effort

Andry Alamsyah, Yahya Peranginangin, Budi Rahardjo, Intan Muchtadi-Alamsyah, Kuspriyanto

Online social media provides platform for social interactions. This platform produce large-scale data generated mostly from online conversations. Network analysis can help us to mine knowledge and pattern from the relationship between actors inside the network. This approach has been crucial in supporting...

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Construction of Tetha-Cyclic Codes over an Algebra of Order 4

Intan Muchtadi-Alamsyah, Aleams Barra, Ahmad Muchlis, Djoko Supriyanto, Irwansyah

In this paper, we show that tetha-cyclic codes over algebra A1 = F2+vF2 can be constructed from binary cyclic codes using a bijection map from A1 to F2 X F2. We also give a decoding

algorithm for tetha-cyclic codes which are constructed using well-known BCH codes over binary field.

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Investigation of H(2H) - Pt(111) Interaction System: using Density Functional Methods

Can Dogan Vurdu, Muhammet Serdar Cavus, Fatma Kandemirli

In this study, interaction system of hydrogen (two hydrogen) with Pt(111) surface has been investigated theoretically by using density functional theory DFT method. With respect to the definitions of interactions of H-Pt(111) and 2H-Pt(111), the potential energy curves PECs belonging to these interactions...

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The Quantum Chemical Calculations of Some Thiazole Derivatives

Murat Saracoglu, Fatma Kandemirli, Mohammed Amin, Can Dogan Vurdu, Muhammet Serdar Cavus, Gokhan Say ner

An examination of quantum chemical and corrosion inhibition studies for some thiazole derivatives, namely 2-amino-4-(p-tolyl)thiazole (APT), 2-methoxy-1,3-thiazole (MTT) and thiazole-4-carboxaldehyde (TCA) had been tested as corrosion safe inhibitors for mild steel (CRS) in 0.5 M H2SO4 solutions at 25...

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Model Identification of Continuous Fermentation under Noisy Measurements

Rudy Agustriyanto

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Surface Interaction between Ethylene, Hydroxide Ion, and Titanium Dioxide Anatase (001): A First Principle Density Functional Theory Study

Paulus Himawan, Mohammad Kemal Agusta, Hermawan Kresno Dipojono, Ganes Shukri, Nugraha

This study covers surface interaction between ethylene, hydroxide ion, and Ti5C adsorption site of titanium dioxide anatase (001). The result of the relaxation suggests that stability was reached on Ti5C site with the adsorption energy of -0.57 eV, while the changes in the bond length and angle between...

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Modeling of Dirac Electron Tunneling Current in Bipolar Transistor Based on Armchair Graphene Nanoribbon Using a Transfer Matrix Method

Endi Suhendi, Rifky Syariati, Fatimah Noor, Neny Kurniasih, Khairurrijal

The Dirac electron tunneling current in an n-p-n bipolar transistor based on armchair graphene nanoribbon (AGNR) has been modeled. The electron wavefunction was derived by employing the relativistic Dirac equation. The transmittance was derived by using the transfer matrix method (TMM). The Landauer...

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Acceleration of norm-conserving Pseudopotential Plane-Wave-Based DFT Calculation on GPU using CUDA

F. Fathurahman, Enngar Alfianto, H. K. Dipojono, M. A. Martoprawiro

In present study, acceleration of density functional theory calculation using norm-conserving pseudopotential and plane wave (NCPP-PW) basis set has been performed. It did not use or parallelize commonly program packages (such as ABINIT, VASP, PWSCF, etc.) but propose prototypical program to carry out...

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Artifacts Removal of EEG Signals using Adaptive Principal Component Analysis

Arjon Turnip, Dwi Esti Kusumandari

Analysis of EEG activity usually raises the problem of differentiating between genuine EEG activity which is introduced through a variety of external influence. These artifacts may affect the outcome of the EEG recording. In this paper, wavelet denoising and band pass filter for preprocessing and an...

Structural Study of Chalcogenide Material Ge-Te-Ga using ab Initio Molecular Dynamics

Lilin Lalita, H. K. Dipojono, M. A. Martoprawiro

Due to its capability of quick amorphous-crystalline phase transition, chalcogenide material Ge-Te-Ga is a potential candidate of a phase change material. For the amorphous phase, the dominant bonding is between Ga and Te. The first peak of Ga-Te bonds is at about 2.7 Å. In the liquid phase, on the other...

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Model Identification of Continuous Fermentation under Noisy Measurements

Rudy Agustriyanto

Chemical Engineering Department, University of Surabaya, Jl. Raya Kalirungkut, Surabaya, Indonesia.

Received: 18 September 2014 / Accepted: 30 November 2014

Abstract:
The dynamic model concept plays a central role in automatic control. Understanding the dynamic behavior of chemical and biological processes depends first on understanding the steady state behavior of these processes, then the dynamic characteristics of the process (e.g., the time constant, gain and deadtime) can be used to determine how long it takes to approach the new steady state and what path the process takes. The dynamic models can be used for bioprocess design, analysis of bioprocess control approaches, operator training, and start-up / shutdown strategy development. This paper will present bioprocess model identification of continuous fermentation for gluconic acid production under measurement noise. In this study, the input and output data was generated from first principle dynamic bioprocess model using Contois kinetic model and mass balances. Simulated measurement noises were then added to process variables. The data was then analyzed using System Identification Toolbox in Matlab. The final results obtained are in the form of Laplace-transfer functions.

Key words: *Biology, chemical, dynamic, laplace, model, simulation*

Introduction

Microbial fermentation is a process in which a population of micro-organism (bacteria, yeasts, moulds, etc) are grown using certain nutritive elements (nutrients) under favorable surrounding conditions (temperature, pH, agitation, aeration, etc). It schematically corresponds to the transformation of subtances (generally carbonaceous substrates) into products, resulting from the metabolic activity of cells. The main components of the reaction are as follows:

- Substrates, denoted as S, which are necessary for the growth of micro-organism, or even which are precursors of a compound to be produced. These substrates generally contain a source of carbon (glucose etc) and sometimes nitrogen and phosphorus.
- Microbial biomasses, denoted as X.
- End products, denoted as P.

From the view point of mathematical modeling, biological reactors can be divided into two major classes: stirred tank reactors (for which the reacting medium is homogenous and the reaction is described by ordinary differential equations), and reactors with a spatial concentration gradient (such as fixed beds, fluidized beds, air lifts, etc., for which the reaction is described by partial differential equations).

In the fermentation of glucose into gluconic acid, the overall reaction mechanism can be described as [1]:

Cell growth:

$$C_6H_{12}O_6 + biomass + O_2 \rightarrow biomass \quad (1)$$

Glucose oxidation:

$$C_6H_{12}O_6 + O_2 \xrightarrow{GOD} C_6H_{10}O_6 + H_2O_2 \quad (2)$$

Gluconolactone hydrolysis:

$$C_6H_{10}O_6 + H_2O \rightarrow C_6H_{12}O_7(GluconicAcid) \quad (3)$$

H_2O_2 decomposition:

$$H_2O_2 \xrightarrow{catalysis} 2H_2O + O_2 \quad (4)$$

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

$$\mu = \mu_m \frac{S}{K_S' X + S} \quad (5)$$

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:

***Corresponding author:** Rudy Agustriyanto,
E-mail: rudy.agustriyanto@staff.ubaya.ac.id

$$\frac{dX}{dt} = r_X = \mu X \quad (6)$$

$$\frac{dS}{dt} = r_S = \frac{1}{Y_{X/S}}\frac{dX}{dt} - \frac{1}{Y_{P/S}}\frac{dP}{dt} - m_S X \quad (7)$$

$$\frac{dP}{dt} = r_P = \alpha\frac{dX}{dt} + \beta X \quad (8)$$

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

The experimental data from batch fermentation and used the data to determine the kinetic parameters by nonlinear least square curve fitting [2] as shown in Table 1.

Table 1. Contois kinetic parameters

Kinetic Parameters	Values	
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}

Simulation

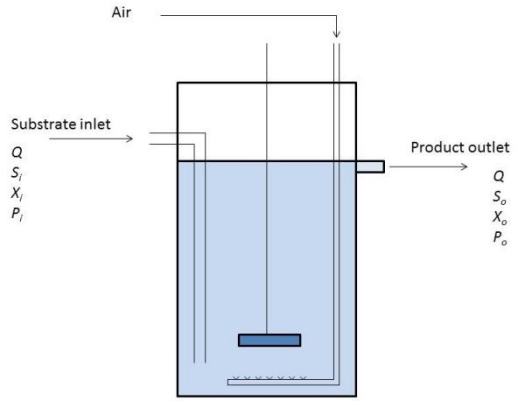

Figure 1. Schematic of continuous fermentation system.

Figure 1 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.

Continuous fermentation as shown in Figure 1 can be modeled based on the mass balance equation of cell, substrate and product [2]. The models are as follows:

$$\frac{dX}{dt}V = QX_i + \frac{\mu_m SX}{K_S^{'}X + S}V - QX \quad (9)$$

$$\frac{dS}{dt}V = QS_i - \left(\frac{1}{Y_{X/S}}\frac{\mu_m SX}{K_S^{'}X + S} + m_S X + \frac{1}{Y_{P/S}}\left(\alpha\frac{\mu_m SX}{K_S^{'}X + S} + \beta X\right)\right)V - QS_o \quad (10)$$

$$\frac{dP}{dt}V = QP_i + \left(\alpha\frac{\mu_m SX}{K_S^{'}X + S} + \beta X\right)V - QP \quad (11)$$

And the steady state operating conditions of continuous fermentation system are shown in Table 2.

Table 2. Steady state operating conditions

Operating Parameters	Values	
Hydraulic retention time, $R=V/Q$	24	h
Inlet cell concentration, X_{iss}	0	
Inlet substrate concentration, S_{iss}	150	g/L
Inlet product concentration, P_{iss}	0	
Outlet cell concentration, Xss	9.3843	g/L
Outlet substrate concentration, S_{ss}	31. 8372	g/L
Outlet product concentration, P_{ss}	0.0863	g/L

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 up and down tests at t=5 hours and t=15 hours were performed for input variables; and measurement noises were added to process outputs.
The complete transfer function expected is in the form [3]:

$$y = G.u \quad (13)$$

where:

$$y = \begin{bmatrix} X \\ S \\ P \end{bmatrix} \quad (14)$$

$$G = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix} \quad (15)$$

$$u = \begin{bmatrix} X_i \\ S_i \\ P_i \end{bmatrix} \quad (16)$$

Results and Discussion

A series of step up and down were performed for all input variables of its nominal steady state at t = 5 h and t=15 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:

$$G = \begin{bmatrix} \frac{0.78288}{2.83535s+1} & \frac{0.063909}{4.1056s+1} & 0 \\ \frac{-0.684}{4.43432s+1} & \frac{0.31143}{0.7449s+1} & 0 \\ \frac{0.0011232}{7.13552s+1} & \frac{0.00069252}{6.2320s+1} & \frac{0.98646}{3.76835s+1} \end{bmatrix}$$

Plots of actual responses and the simulated values using the identified models are shown in Figures 2 to 4. It can be seen from Figures 2 to 4 that the models are satisfactory in that the model simulated values (long range predictions) are very close to the actual process values.

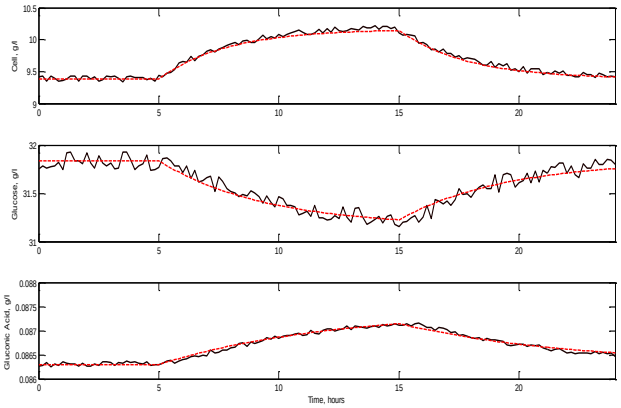

Figure 2. Actual process outputs and the simulated values from the identified model for a unit step up and down of inlet cell concentration at t=5 and t=15 hours. (___ actual values, --- predicted values).

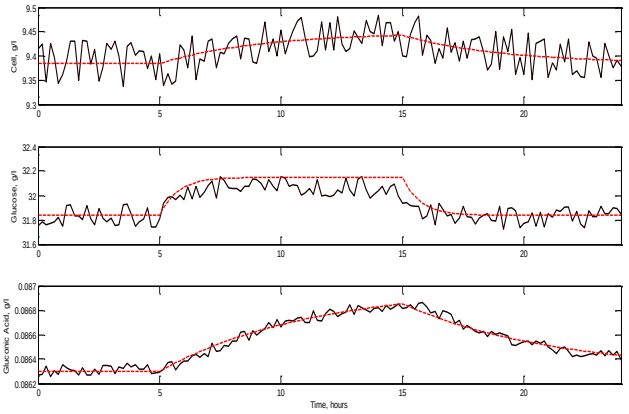

Figure 3. Actual process outputs and the simulated values from the identified model for a unit step up and down of inlet substrate concentration at t=5 and t=15 hours (___ actual values, ---- predicted values).

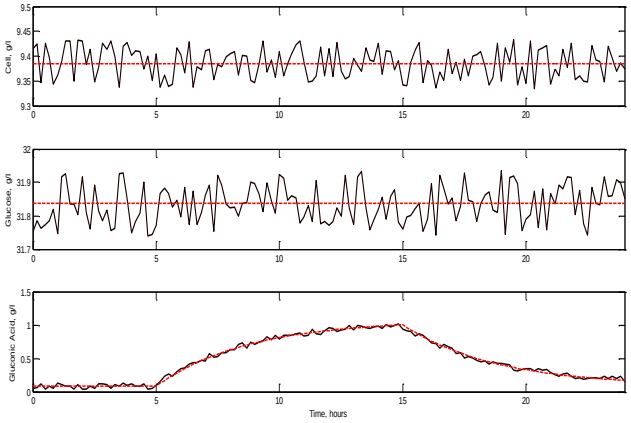

Figure 4. *Actual process outputs and the simulated values from the identified model for a unit step up and down of inlet product concentration at t=5 and t=15 hours (___ actual values, ---- predicted values).*

Conclusions

Model 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.

Acknowledgement

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