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PREFACE

The role of computation and simulation to support research activities in sciences and technologies has become more important in recent decades. The International Conference on Computation in Science and Engineering (ICCSE) 2017 has been conducted in Bandung Institute of Technology (ITB) campus, Bandung, Indonesia, on 10-12 July 2017. This conference is organized by Bandung Institute of Technology (ITB, Indonesia) and supported by UIN Sunan Gunung Jati University. This conference aims at summarizing recent research activities relevant to the computation application in science and engineering and facilitate communication among relevant experts.

More than 150 people from Indonesia, Japan, Malaysia, India, Australia, Korea, and some other countries have participated in this conference. About 150 presentations including 9 plenary talks are presented. The presentations are grouped into 12 areas of particular interest: (1): Complex system Modelling, (2): Energy System Computation, (3): Fluid Dynamics Computation, (4): Artificial Intelligent and Soft Computing, (5): High Energy Physics, (6): Simulation in general, (7): Quantum Computation, (8) HPC, (9): Material Computation, (10): Sub surface modelling and computation, (11): Nuclear and Radiation Computation, and (12): Atmospheric and meteorological computation.

From about 100 full papers submitted after the conference for publication in IOP conference proceedings, after peer review process by relevant experts, 83 papers were accepted for publication in this proceeding. We are indebted to all of authors for submitting their original papers.

We would like to thank all participants, all members of the International Board, members of the Organizing Committee, and I express my gratitude to all those who helped the success of this conference.

Zaki Su'ud

ICCSE 2017 Chairman

Dwi Irwanto

ICCSE 2017 Co-Chairman



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Table of contents

Volume 1090

2018

◀ Previous issue Next issue ▶

International Conference on Computation in Science and Engineering 10-12 July 2017, Bandung, Indonesia

Accepted papers received: 20 August 2018

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[View all abstracts](#)

Preface

OPEN ACCESS 011001
International Conference on Computation in Science and Engineering
+ [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 011002
Peer review statement
+ [View abstract](#) [View article](#) [PDF](#)

Papers

OPEN ACCESS 012001
Current and Future Computation in Nuclear Engineering
Hiroshi Sekimoto
+ [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 012002
By-product group benefits of non-kin resource-sharing in vampire bats
R Donepudi and R Ramaswamy
+ [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

AMIR CPU: World's First and Only 32-bit Softcore Processor in Schematic on Freeware Platform 012003

Muhammad Nasir Ibrahim, Namazi Azhari, Adam Baharum, Mariani Idroas, Uswah Khairudin, Johari Kassim and Mohar Muhammad

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 012004

Effect of isotope enrichment on performance of lead-lithium blanket of inertial fusion reactor

Masatoshi Kondo, Yuu Nakajima, Teruya Tanaka and Takayoshi Norimatsu

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 012005

The Band Structure of a Rare Earth Element of Promethium (III) Oxide (Pm_2O_3) Calculated Using Density Functional Theory

Nur Afifah Mohd Rafi and Ahmad Nazrul Rosli

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 012006

Modified CANDLE Burnup Calculation System, Its Evolution, and Future Development

Zaki Su'ud, M. Ilham, Nina Widiawati and Hiroshi Sekimoto

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 012007

Effects of tangential inlet shape and orientation angle on the fluid dynamics characteristics in a biomass burner

Pasymi, Y W Budhi and Y Bindar

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 012008

Experimental Investigation and Numerical analysis of SO_2 Removal Using Polypropylene Membrane Contactor

D. Ariono, A.N. Hakim and I.G. Wenten

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 012009

Simulation of Semi-Autogenous Grinding (SAG) Mill using Circular-Disks-based Model

R. Sari, P. M. Widartiningsih, M. A. Martoprawiro, L. Hendrajaya and S. Viridi

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS 012010

Analysis, Control and Circuit Design of a Novel Chaotic System with Line Equilibrium

A Sambas, S Vaidyanathan, M Mamat, M Sanjaya WS, S H Yuningsih and K Zakaria

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012011

Comparative Evaluation on Several Reactor Type of Actinide Closed-Cycle Schemes

Sidik Permana, Asril Pramutadi, Syeilendra Pramuditya and Dwi Irwanto

[+ View abstract](#) [View article](#) [PDF](#)

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012012

Experimental and numerical investigation of cooling performance of a cold storage in a pharmaceutical industry

A Sularno, Fxn Soelami and Y Bindar

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012013

Mo-99 Isotope Production Calculation of SAMOP Reactor Experimental Facility

M. Iqbal Farezza W and Syarip

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012014

On The Markov Chain Monte Carlo Convergence Diagnostic of Bayesian Finite Mixture Model for Income Distribution

I Susanto, N Iriawan, H Kuswanto, Suhartono, K Fithriasari, B S S Ulama, W Suryaningtyas and A A Pravitasari

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012015

Numerical Method and Laboratory Experiment of RC Circuit using Raspberry Pi Microprocessor and Python Interface

W. S. Mada Sanjaya, Dyah Anggraeni, Aceng Sambas and Rena Denya

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012016

Finite Difference Methods for Simulation of Water Waves Generated by Moving Topography

Sudi Mungkasi and Nikenasih Binatari

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012017

Approximate Solution of Riccati Differential Equations and DNA Repair Model with Adomian Decomposition Method

Rahmat Al Kafi, Bariqi Abdillah and Sri Mardiyati

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012018

An Evaluation of A Solid Biomass Cook Stove in Small Household Industry

Suhartono, Fitria Gasela, Anis Khoirunnisa and Suharto

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012019

Numerical Study of Radiation Heat Transfer on Supplementary Firing with Gas Turbine Load Variations

Muhammad Haidar Fakhri, A. Teguh Hady and S. Arrad Ghani

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012020

Analysis Service Engineering Development Lifecycle: an Object-Oriented Approach

Ade Hodijah

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012021

Design Study of 600 MWt Long Life Modular Gas Cooled Fast Reactors

M.A. Fareha, Ratna D. Syarifah, Zaki Su'ud and Neny Kurniasih

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012022

Optimization of texture of the multiple textured lubricated contact with slip

M Muchammad, N Sinaga, B Yuniyanto, Arijanto, M F Noorkarim and M Tauviqirrahman

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012023

Solving Unconstrained Global Optimization Problem Using Parameter Free Filled Function in Cooperation with Jameson Gradient Based Method

Herlina Napitupulu, Ismail Bin Mohd, Endang Soeryana Hasbullah, Sukono and Sudradjat Supian

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012024

Design improvement of table fan blade in term of its vibration characteristic using finite element method

O Kurdi, S A Widyanto, A Suprihanto, D B Wibowo, M A Mat Norman and G P Mohana Sundram

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012025

3D simulation of the lubrication film in journal bearing using Fluid-Structure Interaction (FSI)

S Ramdhani, I Haryanto and M Tauviqirrahman

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012026

The application of genetic algorithm optimization on quadratic investment portfolio without a risk-free asset under Value-at-Risk

Sukono, S. Supian, H. Napitupulu, Yuyun Hidayat and Adam Sukma Putra

[+](#) [View abstract](#) [View article](#) [PDF](#)

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012027

Effect of texture shape on the hydrodynamic lubrication performance of the sliding textured contact: a numerical approach

Susilowati, M Tauviqirrahman, J Jamari and AP Bayuseno

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012028

Numerical Study of Nuclear Ground State Properties of Fuel Elements of Nuclear Reactor by Using *Skyrme-Hartree-Fock-Bogoliubov* Method

Yacobus Yulianto, Santi Hatmanti and Zaki Su'ud

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012029

Frontier Orbitals of Dehydrogenated Tetrahydrocurcumin in Water Solvent: A Theoretical Study

Lusia S. P. Boli, Vera Khoirunisa, Adhitya G. Saputro, Mohammad K. Agusta, Febdian Rusydi, Heni Rachmawati and Hermawan K. Dipojono

[+](#) [View abstract](#) [View article](#) [PDF](#)

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012030

Hybrid Cryptosystem Implementation Using IDEA and Knapsack Algorithm for Message Security

Dian Rachmawati, Maya Silvi Lydia and Wynda Arianni Siregar

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012031

Source Term Analysis of SAMOP Reactor Experimental Facility

L Wahid, M I Farezza W and Syarip

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012032

Neutronic Analysis of SAMOP Reactor Experimental Facility Using SCALE Code System

Dedy P Hermawan, Rionaldy and Syarip

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012033

Neutronic Analysis of UN-PuN Fuel use FI-ITB-CHI Code for 500MWth GFR Long Life Without Refueling

Ratna Dewi Syarifah, Zaki Su'ud, Khairul Basar and Dwi Irwanto

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012034

Small Signal Stability Analysis of Wind Turbine Penetration in Sulselrabar Interconnection System

B Mustadir Darusman, Ansar Suyuti and Indar Chaerah Gunadin

[+](#) [View abstract](#) [View article](#) [PDF](#)

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012035

Expansion of Filter Design from GHz to THz with Metamaterial Hexagonal Split Ring Resonator

M. F. Kurnia, R.F. Syahputra and Saktioto

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012036

Analytical Method of Atomic Density Determination of Uranyl Nitrate Solution

Syarip and Tegas Sutondo

[+](#) [View abstract](#) [View article](#) [PDF](#)

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012037

Driver Drowsiness Detection Based on Face Feature and PERCLOS

Suhandi Junaedi and Habibullah Akbar

[+](#) [View abstract](#) [View article](#) [PDF](#)

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012038

Dynamics, Circuit Design and Fractional-Order Form of a Modified Rucklidge Chaotic System

A Sambas, S Vaidyanathan, M Mamat, M Sanjaya WS, S H Yuningsih, K Zakaria and Subiyanto

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012039

Evaluation of downscaled near-surface wind over maritime continent based on stations measurement

Arnida L. Latifah, Aryo Cokrowatianto and Didit Adytia

[+](#) [View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012040

Optimization of time-dose fractionation radiotherapy scheme by simulated annealing with consideration of biological factor

A N Hasto and W Rena

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012041

Inertia effect of textured lubricated contact on the bearing performance using CFD approach

F Hilmy, M Muchammad, M Tauviquirrahman and J Jamari

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012042

Numerical evaluation of number of textures in slip-textured lubricated contact

E Yohana, W K Ajie and M Tauviquirrahman

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012043

Intelligent Software Product Line For Supply Chain

Ahmad Nurul Fajar, Ditdit Nugeraha Utama and Gunawan Wang

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012044

Design of Real Time Facial Tracking and Expression Recognition for Human-Robot Interaction

W.S. Mada Sanjaya, Dyah Anggraeni, Atip Juwardi and Madinatul Munawwaroh

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012045

The effect of heterogeneity in ion-exchange membrane structure on Donnan Exclusion

K. Khoiruddin, Danu Ariono, S. Subagjo and I Gede Wenten

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012046

Speech Recognition using Linear Predictive Coding (LPC) and Adaptive Neuro-Fuzzy (ANFIS) to Control 5 DoF Arm Robot

W.S. Mada Sanjaya, Dyah Anggraeni and Ikhsan Purnama Santika

[+ View abstract](#) [View article](#) [PDF](#)

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012047

A finite volume method for solving the gravity wave-model equations

Cecilia Heru Purwitaningsih and Sudi Mungkasi

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012048

Inverse Modeling of Gravity Data with Two Layers Density in Sedimentary Basin Structure

OPEN ACCESS

012049

Comparison of absorbed dose distribution 10 MV photon beam on water phantom using Monte Carlo method and Analytical Anisotropic Algorithm

Ridwan Ramdani, Freddy Haryanto and Yudha Satya Perkasa

OPEN ACCESS

012050

Numerical solutions to a parabolic model of two-layer fluids

Sudi Mungkasi and Friska Dwi Mesra Mangadil

OPEN ACCESS

012051

Vortex Formation on Horizontal Axis Wind Turbine with Splitted winglets

Rizal Ibnu Syifa and Setyo Nugroho

OPEN ACCESS

012052

Analysis of Fouling Mechanism in Polysulfone based Ultrafiltration Membrane during Peat Water Filtration

Danu Ariono and Anita Kusuma Wardani

OPEN ACCESS

012053

In Silico Study of Phospholipids as An Oral Insulin Delivery System

Nanik Rahmawati Fuadah and Rukman Hertadi

OPEN ACCESS

012054

Ab Initio Study on Electronic Structure of Some Imidazole Derivatives and Its Correlation with Corrosion Inhibition Properties

C D D Sundari, S Setiadji, B W Nuryadin, R Syafia, A F Huda and A L Ivansyah

OPEN ACCESS

012055

Computational Study of Inclusion Complexes Between Omeprazole Enantiomer with Hydroxypropyl- β -Cyclodextrin

S Setiadji, C D D Sundari, B W Nuryadin, H Zayyinnisya, R Cahyandari and A L Ivansyah

OPEN ACCESS

012056

The reasoning for low ground magnetic anomaly reveal by model numeric and data on the field

Agus Laesanpura, Warsa and S. Tedy

[+](#) View abstract [View article](#) [PDF](#)

OPEN ACCESS

012057

Alternating Least Square Method for Decomposing Dance Golek Menak Tensor Data

Joko Sutopo

[+](#) View abstract [View article](#) [PDF](#)

OPEN ACCESS

012058

Influence of Electrical Properties on Radiation and Emission to Pinch Radius Thermal Plasma Device

R F Syahputra, R Farma, Saktioto, N D Nawi, N A Rashid, F D Ismail and J Ali

[+](#) View abstract [View article](#) [PDF](#)

OPEN ACCESS

012059

Service Desk Implementation with Information Technology Infrastructure Library Framework (Study Case Financial Company)

Dwi Handoko and Abba Suganda Girsang

[+](#) View abstract [View article](#) [PDF](#)

OPEN ACCESS

012060

Evaluation of ISO 27001 implementation towards information security of cloud service customer in PT. IndoDev Niaga Internet

Ahmad Nurul Fajar, Hendy Christian and Abba Suganda Girsang

[+](#) View abstract [View article](#) [PDF](#)

OPEN ACCESS

012061

Fuel Breeding Analysis On Low Moderated Fuel Ratio Based On Actinides Closed Water-Cooled Thorium Reactor

Sidik Permana, Syeilendra Pramuditya and Dwi Irwanto

[+](#) View abstract [View article](#) [PDF](#)

OPEN ACCESS

012062

Implementation of Rivest Shamir Adleman Cryptographic Algorithms and Techniques of Steganography First of File for Message Security

Dian Rachmawati and Yeni Rosalin Munthe

[+](#) View abstract [View article](#) [PDF](#)

OPEN ACCESS

012063

Isogeometric Analysis for Thin Square Bending Plate using Collocation Method

Irwan Katili, Budiarto Jaya, Imam Jauhari Maknun and Mulia Orientilize

[+](#) View abstract [View article](#) [PDF](#)

-
- OPEN ACCESS** 012064
Numerical Simulation on Solving Three-Dimensional Global Optimization Problems in cooperation of Filled Function and Search Direction
Herlina Napitupulu, Ismail Bin Mohd, Yuyun Hidayat, Sukono and Sudradjat Supian
[+](#) View abstract [View article](#) [PDF](#)
-
- OPEN ACCESS** 012065
Numerical simulation of breaking regular and irregular wave propagation above a sloping bottom
Didit Adytia, Semeidi Husrin and Adiwijaya
[+](#) View abstract [View article](#) [PDF](#)
-
- OPEN ACCESS** 012066
Thermal analysis of composite disc-brake based on finite element method
S Riyadi, Sulistyono and M Tauviquirrahman
[+](#) View abstract [View article](#) [PDF](#)
-
- OPEN ACCESS** 012067
CFD analysis of texture depth effect on the performance of hydrodynamic lubricated bearing
M Muchammad, F Hilmy, M Tauviquirrahman, J Jamari and DJ Schipper
[+](#) View abstract [View article](#) [PDF](#)
-
- OPEN ACCESS** 012068
Numerical optimization of load support of the single textured lubricated contact with boundary slip
M Tauviquirrahman, M F Noorkarim, Arijanto and Muchammad
[+](#) View abstract [View article](#) [PDF](#)
-
- OPEN ACCESS** 012069
Optimization of Enemy's Behavior in Super Mario Bros Game Using Fuzzy Sugeno Model
Nanang Ismail, R M Husnul, M Nurul Subkhi, Miftahudin and Eki A Z Hamidi
[+](#) View abstract [View article](#) [PDF](#)
-
- OPEN ACCESS** 012070
Colored Object Sorting using 5 DoF Robot Arm based Artificial Neural Network (ANN) Method
W. S. Mada Sanjaya, Dyah Anggraeni, Madinatul Munawwaroh, M. Yusuf S. Nurasyidiek, Darmawan Setia Rahayu, Ahmad Samsudin, Ikhsan Purnama Santika and Endah Kinarya Palupi
[+](#) View abstract [View article](#) [PDF](#)
-
- OPEN ACCESS** 012071

Neutronic Comparison Study Between Pb(208)-Bi and Pb(208) as a Coolant In The Fast Reactor With Modified CANDLE Burn up Scheme.

Nina Widiawati, Zaki Suud, Dwi Irwanto and Hiroshi Sekimoto

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012072

On The Bernoulli Mixture Model for Bidikmisi Scholarship Classification with Bayesian MCMC

W Suryaningtyas, N Iriawan, K Fithriasari, BSS Ulama, I Susanto and AA Pravitasari

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012073

Preliminary Study of Long-life GFR 100 and 150 MWth

S.C. Pattipawaej and Z. Su'ud

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012074

Flory-Huggins Based Model to Determine Thermodynamic Property of Polymeric Membrane Solution

P T P Aryanti, D Ariono, A N Hakim and I G Wenten

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012075

Tidal Current Circulation in Western Bali Sea Using a 2-D Hydrodynamic Model

D A Widiawan and S Nurdjaman

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012076

Optimizing and Implementation Contactless Tag-Reader System for Smart Classroom and Laboratory Access

Rida Ariyanti, Elyas Palantei and Intan Sari Areni

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012077

The Effect of Grounding Resistance About Back Flashover on 150 KV Transmission Network in Main Station of Sungguminasa - Tallasa (Makassar)

Naomi Lembang, Salama Manjang and Ikhlas Kitta

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012078

A Numerical Investigation of the Friction Contact of an Unfilled Styrene Butadiene Rubber by a Blade Sliding Indentation

B. Setiyana, M. Khafidh, R. Ismail, J. Jamari and D.J. Schipper

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012079

Design Project Management System Based on SOA Approach

Abba Suganda Girsang, Fahmi Jafar and Ahmad Nurul Fajar

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012080

The *Hybrid* Model Algorithm on Sharia Insurance

Rini Cahyandari, Riva Lesta Ariany, Sukono and Yudha Satya Perkasa

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012081

Development of Ebola Vaccine Candidate by in Silico from Glikoprotein (GP) Gene of Ebola Zaire Virus

Yani Suryani, Opik Taupiqurrohman, Sri Aryanti, Moh. Nurul Subkhi and Epa Paujiah

[+ View abstract](#) [View article](#) [PDF](#)

OPEN ACCESS

012082

Appropriateness of Water Hyacinth and Rice Husk as Filler Materials for Resin Polymer Insulation

Trisna Amelia Fitriah, Salama Manjang and Ikhlas Kitta

[+ View abstract](#) [View article](#) [PDF](#)

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Frontier Orbitals of Dehydrogenated Tetrahydrocurcumin in Water Solvent: A Theoretical Study

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Abstract. We studied two frontier orbitals - the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO)- of tetrahydrocurcumin (THC) using density-functional theory (DFT) in water solvent. These orbitals were observed in THC molecule without one hydrogen atom (dehydrogenated THC). The loss of hydrogen atom is due to the transfer of the atom from THC molecule toward reactive oxygen species (ROS) (Hydrogen atom transfer –HAT- mechanism). We began our investigation by optimizing dehydrogenated THC at three X-H sites. Then, water solvent was added by using polarized continuum model (PCM) method. This study observed that dehydrogenated THC at two O-H sites has wider gap of HOMO-LUMO compare to C-H site.

1. Introduction

Studying dehydrogenation of THC is an initial step to understand the role of THC as antioxidant based on hydrogen atom transfer (HAT). In biological system, excessive amount of reactive oxygen species (ROS) promotes oxidative stress [1]. Thus, THC is proposed as one of the antioxidant agents that can prevent oxidative stress in biological system. In playing its role, THC is expected to transfer one of its hydrogen atom toward ROS to neutralize the free radical molecule[2]. This is called hydrogen atom transfer mechanism. Due to HAT mechanism, THC is left with one less hydrogen atom or so called dehydrogenated THC. A good antioxidant agent is expected to maintain the stability of its dehydrogenated form[3].

There are two frontier orbitals used to assess stability of dehydrogenated THC. They are the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). Gap between this two orbitals will decide the ability of electrons to jump from HOMO to LUMO. Wide gap means is correlated to high stability while narrow gap is correlated to low stability[4].

In this research, we intend to study two frontier orbitals of THC produced by THC dehydrogenated using first principles. We choose density functional theory (DFT) as our research framework since it can produce frontier orbitals of dehydrogenated THC by constructing electronic structures only. Thus



this is called first principles study. Result of this study will guide us to decide the stability of dehydrogenated THC after transferring a hydrogen atom from an X-H site. We analyze the HOMO and LUMO energy of three X-H sites of THC to lead us to our final conclusion. THC performs better antioxidant reactivity in polar medium [5], so we choose polar water medium as our simulation environment. We are aware of the problematic of PCM in modeling water as solvent in our previous works where the trend predicted by DFT-PCM calculations always break when using water solvent [6,7].

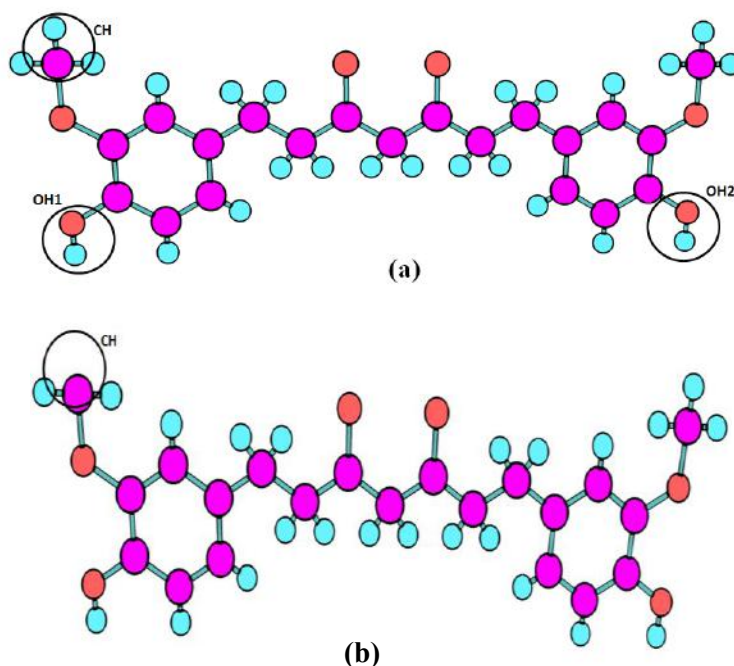


Figure 1. Molecular geometry of (a) THC molecule and (b) dehydrogenated THC produced by abstracting a hydrogen atom from CH site.

2. Computational details

We performed geometry optimization of three THC radicals at site OH1, OH2 and CH using UM05-2X functional and 6-31++G(d,p) basis set. Some authors have successfully used M05-2X functional to study the antioxidant properties of polyphenols [8, 9]. The developer of this functional was also suggesting it for thermochemistry calculations [10]. Since our system was an open shell system of THC dehydrogenated, we performed an unrestricted calculation. Our simulation was done in water environment to represent a polar medium. This solvent effect was included using polarized continuum model (PCM), where water was modelled as cavity that interacts electrostatically with THC radical placed within the cavity [11]. All calculations were performed using Gaussian 09 suite program [12] at 298.15 K.

3. Results and discussion

Figure 1(a) shows model of our molecule of interest which is a THC molecule. Site CH, OH1 and OH2 mark three targeted sites with the ability of transferring a hydrogen atom. We abstract one hydrogen atom from each of this site respectively to create dehydrogenated THC. Figure 1(b) shows

dehydrogenated THC at C-H site. Our DFT calculations coupled with PCM confirms that the geometry of our system is in minimum energy with doublet spin states.

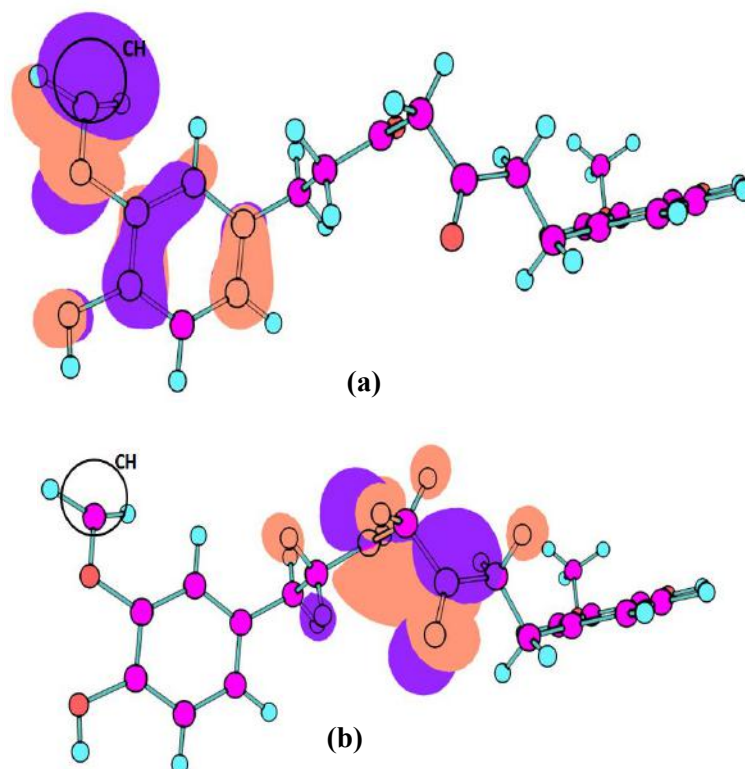


Figure 2. (a) HOMO and (b) LUMO profiles of dehydrogenated THC at CH site.

Figure 2 presents HOMO and LUMO profiles of dehydrogenated THC at C-H site. As shown in 2(a), the HOMO profile is located at dehydrogenated site while in 2(b), the LUMO profile is located in the middle of the molecule. This result is also true for site OH1 and OH2.

Figure 3 summarizes the relative HOMO-LUMO energy of our three dehydrogenated THC systems. In general, O-H sites have higher relative HOMO-LUMO energy than CH site. Higher relative HOMO-LUMO energy means electrons cannot jump easily from HOMO to LUMO. As a result, dehydrogenated THC at O-H sites is more stable than at C-H sites. Site OH1 and OH2 possess very similar value of relative energy HOMO-LUMO. This result predicts that hydrogen atom transfer from both sides will produce the same stability of dehydrogenated THC in water environment. We compare our results to one of our previous work for relative HOMO-LUMO of THC in gas phase [13] and conclude that water solvent does not affect the stability of dehydrogenated THC.

4. Conclusion

The study of frontier orbitals of dehydrogenated THC in water solution showed that when hydrogen atom transfer occurred at O-H site, the stability of dehydrogenated THC is higher than when it occurred at C-H site. Hydrogen atom transfer at two O-H sites in THC will produce dehydrogenated THC with the same stability.

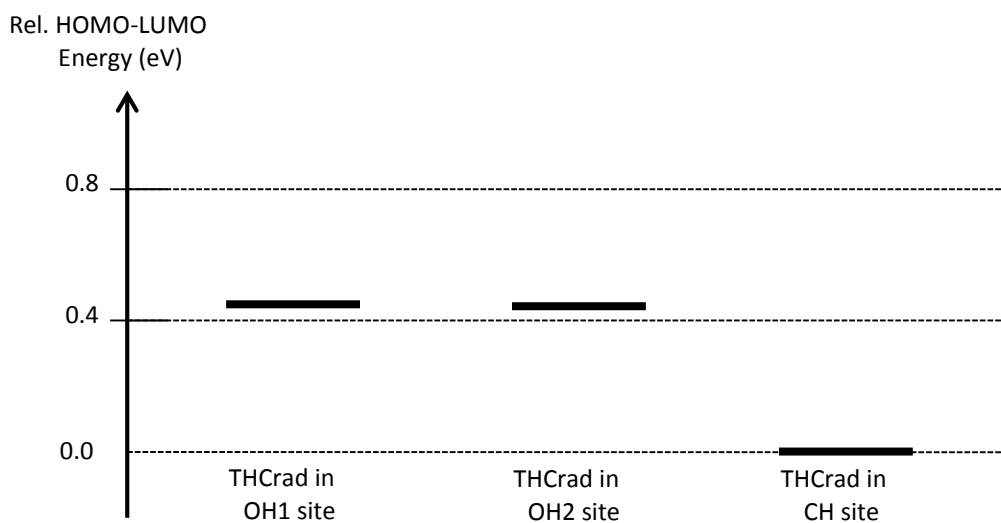


Figure 3. Relative energy diagram of THC radicals in OH1, OH2 and CH sites

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