

## ***MATHEMATICAL, PHYSICAL AND ENGINEERING SCIENCES***

### **83. MEASUREMENT OF THE W BOSON MASS USING THE JLC STUDY FRAMEWORK (JSF)**

DENNIS C. AROGANCIA<sup>1</sup>, ALLISTER LEVI C. SANCHEZ<sup>1</sup>,  
JINGLE B. MAGALLANES<sup>1</sup>, HERMOGENES C. GOOC<sup>1</sup>,  
ANGELINA M. BACALA<sup>1</sup>, KEISUKE FUJII<sup>2</sup>, and  
AKIYA MIYAMOTO<sup>2</sup>

<sup>1</sup>*Department of Physics, Computational High Energy Physics Laboratory,  
Mindanao State University-Iligan Institute of Technology,  
9200 Iligan City*

<sup>2</sup>*Institute of Particle and Nuclear Science, KEK,  
Tsukuba, Japan 305*

The Standard Model (SM) asserts that the matter is ultimately composed of three generations of pointlike particles called quarks and leptons and their intermediary particles called gauge bosons; all of which have been directly observed to date except for the Higgs boson. To search for this elusive particle, the Asian high energy physics community has proposed a next-generation linear accelerator facility to be built in Japan called the Joint Linear Collider (JLC) which runs at center-of-mass energies of 500 GeV to 1.5 TeV.

Since the Higgs boson is sensitive to the precision measurements of the weak bosons, we investigated the reaction  $e^+e^- \rightarrow evW$  using computer simulation work at MSU-IIT Computational Physics Laboratory. Events from this reaction were generated and analyzed by using the JLC Study Framework (JSF); a software library based on the ROOT suite of programs provided by the European high energy physics laboratory called CERN. In running JSF, other software libraries were installed such as CERNLIB, ROOT, and LCLIB; all from CERN and the PHYSSIM library by KEK physicists. Default configurations of the JLC detectors

such as the different *vertex detectors, central drift chamber, calorimeter, muon detector, and superconducting solenoid magnet* were already set in the simulation; so with the 3 Tesla detector parameter setting.

Measurement of the W boson mass used the semileptonic channel particularly  $e^+e^- \rightarrow evW$  because it has a larger cross section and does not have an ambiguity due to final state color exchange in 4 jets final state. Event generation and simulation used the packages called *BASES/SPRING* and *JSF Quick Simulator* respectively with a center of mass energy set at 500 GeV. Data analysis used graphical user analysis (GUI) which include effects from *initial state radiation (ISR)* and *beamsstrahlung*. Calculation of total cross section in such process was done in using *BASES*. W mass was measured directly from its decayed products, particularly quarks. In the event selection criteria, neutrinos were removed and all particles that went into the beam pipe direction. Theoretically, the mass of the W boson is about 80 GeV which was used as input mass in the computer simulation. In this paper the mass of the W boson was measured to be 80.41 GeV with ISR effects and 80.40 GeV with beamsstrahlung effects. Based on this result the relative error is less than 1%.

**Key words:** standard model, JLC Study Framework (JSF), ROOT, LCLIB, CERNLIB, PHYSSIM, JSF, quick simulator, BASES/SPRING, ISR, beamsstrahlung

## 84. POLYTHIOPHENE AND POLYPYRROLE THIN FILMS AS RADIATION SENSORS

ARNOLD C. ALGUNO<sup>1</sup>, ROLANDO V. BANTACULO<sup>1</sup>, ANCELIE CASTILLON<sup>1</sup>, ANGELINA M. BACALA<sup>1</sup>, HITOSHI MIYATA<sup>2</sup>,  
and BIOGROUP<sup>2</sup>

<sup>1</sup>*Department of Physics*

*Mindanao State University-Iligan Institute of Technology, 9200 Iligan City*

<sup>2</sup>*Department of High Energy Physics, Niigata University  
Niigata City, Japan*

Radiation detectors play a vital role in understanding what makes up matter and in the development of various fields of science especially in medical and physical sciences. The most commonly used material in radiation detectors is silicon (Si) which provides high efficiency in radiation detection.

However, when the large detector is needed, Si cannot be used because it is too difficult to make large silicon crystals, and it is also very expensive to make a large silicon semiconductor detector.

This research explored the possibility of using conducting polymers that are organic semiconductors as radiation sensors that could replace silicon.

Polythiophene and polypyrrole thin freestanding films were prepared through electrochemical polymerization by passing a constant electric potential across indium-tin oxide and platinum-plated titanium plate electrodes. These electrodes were immersed in an electrolytic solution containing thiophene and pyrrole, lithium tetrafluoroborate (electrolyte salt) and acetonitrile (solvent). The resulting films were dedoped in pure acetonitrile at a higher negative bias potential for a longer time. Polypyrrole and polythiophene sensors were fabricated using the corresponding thin films prepared. Aluminum mylar sheets and gold sheets were attached to both ends of the sensors that served as electrodes. The voltage-current (V-I) curves showed evident responses when they irradiated with ultraviolet (UV) light illumination, Strontium 90 ( $^{90}\text{Sr}$ ) beta ray and Nd:YAG laser. Signals coming from these sensors established good ohmic relationship and conductivities were found to be in the orders of magnitude of  $10^{-10}$  to  $10^{-5}$  S.cm $^{-1}$ . This study shows that signals obtained with the polymers were similar to those from using Si-PIN photodiode.

**Key words:** radiation sensor, dopant concentration, conductivity, polythiophene, Polypyrrole, tetrafluoroborate, solvent, electropolymerization, freestanding film, conducting polymer

## 85. MOSFET DOSIMETRY FOR RADIOTHERAPY INTERFACE MEASUREMENTS

GERARD BENGUA<sup>1</sup>, ANATOLY ROZONFELD<sup>2</sup>,  
and PETER METCALFE<sup>2,3</sup>

<sup>1</sup>*Physics Department, De La Salle University  
2401 Taft Avenue, 1004 Manila*

<sup>2</sup>*Engineering Physics Department, University of Wollongong  
New South Wales, Australia*

<sup>3</sup>*Illawarra Cancer Care Center, Wollongong  
New South Wales, Australia*

An n-channel Metal Oxide Semiconductor Field Effect Transistor (MOSFET) was used to investigate the dose distribution near interfaces. The MOSFETs were irradiated in  $5 \times 5 \text{cm}^2$  and  $10 \times 10 \text{cm}^2$  radiation field with 6MV x-rays and 12MeV electron beams from a Varian 2100c linear accelerator. The dosimeters were operated in an active mode, biased gate, during irradiation. Two different air cavity geometries were modeled using solid water sheets. An Attix chamber and

sheets of Gafchromic films were used to measure the dose near and at the interfaces. Results obtained by these detectors were used as benchmarks for data comparison. Additionally the results from an ADAC-Pinnacle dose planning system and EGS4 Monte Carlo simulation of the dose build up and build down effects for tissue-air-tissue and tissue-lung interfaces have been simulated.

Dose measurements for tissue-lung interface were carried out using an anthropomorphic phantom made from plastic water and inserts of lung phantom material. Depth increments of as small as 100 $\mu$ m enabled the detailed measurement of dose at the interfaces by utilizing the MOSFET dosimeter. In all cases, the effects of the loss of electronic equilibrium and the reduced backscatter due to the existence of inhomogeneities were shown.

Interface dose distributions obtained by the MOSFET dosimeters were within 5% to 6% of the results of the Attix chamber measurements and Monte Carlo-EGS4 simulation results. Comparison of the dose distributions near interfaces generated by the ADAC-Pinnacle planning computer system and those experimentally measured showed that the former overestimates the dose near the interface (<2mm from interface) by around 7% for small cavity sizes (2x2x30cm<sup>3</sup>) irradiated with 5x5cm<sup>2</sup> field size and about 12% for a larger cavity sizes (2x2x30cm<sup>3</sup>) using the same field size.

Present inhomogeneity correction algorithms have been found to predict dose distributions where tissue-lung interface is involved to a reasonable accuracy (3%) compared with experimental results.

The good agreement between the data obtained by the MOSFET with that of Attix chamber, Radiochromic film and Monte-Carlo EGS4 simulated data indicated the viability of its use as a clinical dosimeter for interface dose measurements.

**Key words:** MOSFET, interface, inhomogeneity, Monte-Carlo EGS4, planning computer, radiochromic film, dosimeter, dose, cavity, Attix chamber

## 86. MEAN LIFETIME MEASUREMENT OF THE 14 keV STATE IN THE TRANSITION OF <sup>57</sup>Co to <sup>57</sup>Fe

MERLITA C. GARCIA<sup>1</sup> and ANGELINA M. BACALA<sup>2</sup>

<sup>1</sup>*Ateneo de Zamboanga, Arts and Sciences Division  
Zamboanga City*

<sup>2</sup>*Department of Physics, Mindanao State University-  
Iligan Institute of Technology  
9200 Iligan City*

In the beta decay of <sup>57</sup>Co to <sup>57</sup>Fe, the de-excitation of the second excited state to the first excited state gives off a 122 keV gamma ray photon while the de-excitation of the first excited state to the ground state gives off a 14 keV gamma

ray photon. In this decay made the emission of the gamma photons are in cascade and are then considered to be coincident. Lifetime measurement uses the principle of the method of coincidence.

Two different detectors were used: a 2" in diameter by 2" thick scintillator to detect the 122 keV gamma photon and a 1" in diameter by 0.25" thick scintillator to detect the 14 keV gamma photon. Using the Nuclear Instrumentation Modules (NIM) and the Computer Automated Measurements and Control (CAMAC) modules such as the Analog to Digital Converters (ADC) and the Time to Digital Converters (TDC) with their proper calibrations, and a macro in fortran, the energy spectrum of the particles of interest incident on these detectors were viewed in the monitor of a personal computer and the time between the detection of these two energies determined. The ADC and the TDC spectra were analyzed using the ROOT data analysis system for histogramming and fitting.

Results showed that the individual time spectrum for each set of data taken on different times gave a mean lifetime value for the 14 keV state which agrees well with an internationally accepted value of 141 ns.

From these results it can be seen that Nuclear Instrumentation Modules (NIM) and the Computer Automated Measurement and Control (CAMAC) modules available at the MSU-IIT High Energy Physics Laboratory are capable of measuring lifetimes of nuclear states which are less than a second.

**Key words:** lifetime, gamma photons, scintillator, photomultiplier, NIM, CAMAC, ADC, TDC, energy spectrum, time spectrum

## 87. BILINEAR HENSTOCK-STIELTJES INTEGRAL

FERDINAND P. JAMIL<sup>1</sup> and SERGIO R. CANOY, JR.<sup>2</sup>

<sup>1</sup>*Department of Mathematics, Mindanao State University-Main  
Marawi City*

<sup>2</sup>*Department of Mathematics  
Mindanao State University-Iligan Institute of Technology  
9200 Iligan City*

Both the bilinear Riemann-Stieltjes and Moore-Pollard-Stieltjes integrals have certain difficulties and shortcomings in the case where the functions under the integral sign share a common discontinuity. To overcome some of the deficiencies of these integrals, a new integration process must be developed. In 1995, the second author introduced the bilinear Henstock-Stieltjes integral for Banach-valued functions and proved the existence of the integral in the case where the function is continuous and the integrator is of bounded variation or bounded semi-variation. Recently, these authors proved the existence of the same integral in the case

where the function is regulated and the integrator is of bounded variation. Indeed, as seen and proved, the Henstock-Stieltjes integral is far better and has greater advantage than the former aforementioned integrals. In fact, as an example will show, the condition that the integrator be of bounded variation is not even necessary for the existence of the integral. Furthermore, this paper offers two main results, namely, the existence of the bilinear Henstock-Stieltjes integral in the case where the functions are both regulated and a better integration by parts formula.

## 88. THE SMALLEST NON-ASSOCIATIVE INVERSE PROPERTY LOOP AND SOME GENERALIZATIONS

ALEXANDER S. CARRASCAL

*ECE Department, College of Engineering*

*Polytechnic University of the Philippines, Sta. Mesa, Manila*

The smallest non-associative loop with *inverse property (IP)* is of order 7. Up to isomorphism, this is the only IP loop of that order. This unique loop possesses interesting properties that can be generalized for the construction of IP loops of higher order. These generalizations led to the discovery and construction of several special families of IP loops in which the IP loop of order 7 is the smallest member. These special families include IP loops of order (1)  $n = 3m - 2$ ,  $m \geq 3$ ; (2)  $n = 4m - 1$ ,  $m \geq 2$ , and (3)  $n = 2^k - 1$ ,  $k \geq 3$ . The properties of the IP loops of order  $n = 3m - 2$  and  $n = 2^k - 1$  can be combined together to construct an IP family of order  $n = (2^k - 1)m - 2^k + 1$ , where  $k \geq 3$  and  $m \geq 3$ . Moreover, each of these families could be further generalized to construct other families of IP loops. Finally, a particular member of one family can be used as a subloop in the construction of a higher order member of that family or another family.

**Key words:** non-associative loop, inverse property (IP)

## 89. ON CAYLEY ALGEBRAS OF DIMENSION $2^r$ , $r \geq 4$

RAOUL E. CAWAGAS

*SciTech R&D Center*

*Polytechnic University of the Philippines, Sta. Mesa, Manila*

The existence of *Cayley Algebras of Dimension  $n = 2^r$*  is established by construction using a new procedure called the *ZSM Process*. These algebras form a class of flexible real algebras that includes the *Cayley-Dickson algebras* as a subclass. If  $r \geq 4$ , one of the smallest algebras of this type is the *sedenions*  $S$  ( $n = 2^4$ ) which contains as subalgebras the *real numbers*  $R$  ( $n = 2^0$ ), *complex numbers*

$C$  ( $n = 2^1$ ) quaternions  $H$  ( $n = 2^2$ ), all of which are associative, and the Cayley numbers (octonions)  $O$  ( $n = 2^3$ ) which is nonassociative. This paper shows that these real algebras have a common structural base (the Klein group of order  $n = 2^r$ ), and they all belong to a single family composed of classes of Cayley algebras of dimension  $2^r$ .

**Key words:** Cayley-Dickson algebras, ZSM process, sedenions, octonions, quaternions

## 90. DETERMINATION OF ALL ELEMENTARY NAFIL LOOPS OF ORDER 7

RENILDA S. LAYNO

*SciTech R&D Center*

*Polytechnic University of the Philippines, Sta. Mesa, Manila*

The study of *NAFILs* (*non-associative finite invertible loops*) is a new frontier in the theory of loops and quasigroups. This is a class of loops that includes the familiar IP, Moufang, and Bol loops which are involved in such diverse fields as finite geometries, combinatorics, and theoretical physics. Not much is known about other interesting loops in this class like the *elementary* NAFILs (loops with no non-trivial subsystem).

This paper deals with the study of elementary NAFIL loops of small order. In particular it presents studies on the determination of all elementary NAFIL loops of order  $n = 7$  using the software FINITAS. This software was developed as a tool for the analysis and construction of finite algebraic structures.

The results show that there are exactly 2,333 NAFIL loops of order  $n = 7$  out of which 16 are abelian and 2,317 are non-abelian. Out of the 16 abelian NAFILs, 8 are elementary. Of the 2,317 non-abelian elementary NAFILs, exactly 681 have one self-inverse element. To date we have determined about 176 non-abelian elementary NAFILs of order 7. Most of these elementary NAFILs have Cayley table that are full permutations. Moreover, many of these have no known loop properties like IP (inverse property), AP (alternative property), CIP (cross-inverse property), etc. The search for other elementary NAFILs of order 7 is still continuing.

**Key words:** loop, non-associative, invertible, NAFIL, elementary, FINITAS

## 91. SSADM SYSTEM DATA MODELER: A DATA MODELING TOOL

MA. SHIELA A. MAGBOO

*Department of Physical Sciences and Mathematics  
College of Arts and Sciences, University of the Philippines Manila  
Padre Faura, Ermita, Manila*

Data models help ensure a good database design. However, most data modeling tools are either pure data modeling tools or have some sort of integration but is too costly for most people. To solve this problem, the author created SSADM System Data Modeler, a computer-aided software engineering (CASE) tool that supports both top-level and bottom-level approach to data modeling. The tool conforms to the notations used in Structured Systems Analysis and Design Method (SSADM) Version 4+, a technique popular in the United Kingdom that supports the analysis and design phases of information systems development [Goodland, 1995].

The objective of this study is to identify the basic data modeling features that data designers look for and to show that SSADM System Data Modeler satisfies most of these basic features.

The author enumerated the list of data modeling features of SSADM System Data Modeler and tested each to verify that the tool is indeed capable of performing the indicated features. These features include the ability to (a) create data representation using Logical Data Models (LDM) consistent with the syntactical rules of specific method, in this case SSADM; (b) edit description about entities, relationships and attributes which further illustrate the objects, their properties and interrelationships with other objects; (c) perform normalization up to Third Normal Form; (d) integrate the results of top-level and bottom-up approach to data analysis; (e) provide consistent environment to prevent the user from performing invalid actions; (f) create the database structure of the corresponding diagram in MS Access; (g) automatically update the diagram and corresponding database whenever an operation such as create, edit or delete of entities, relationships or attributes is performed; (h) generate error messages in case of diagram inconsistencies; (i) help facilitate to describe how to use the software; (j) print the diagram as well as other documents supporting the diagram.

SSADM System Data Modeler satisfies most of the expectations, however, it falls short on the following aspects: (a) database platform it creates; (b) its inability to convert a legacy database to another platform; (c) the notation it supports; and (d) the number of users it accommodates. Although it has a capability to create a database structure from the resulting diagram, the resulting database platform is limited to Microsoft Access. It has no reengineering features to convert a legacy database into another platform. It supports only one notation, the SSADM notation, which is not as widely used as the other notations. It does not support the Unified Modeling Language (UML) notation which is the de facto standard



for object-oriented analysis and design. It is also stand-alone, not multi-user like what most data designers want. However, despite all these limitations, SSADM System Data Modeler is still able to accomplish most of the features of a basic stand-alone data modeling tool. The resulting software can then be refined later to address most, if not all the identified limitations.

**Key words:** data modeling, computer-aided software engineering (CASE), Logical Data Structure (LDS), Logical Data Model (LDM), Entity Relationship Diagram (ERD), Structured Systems Analysis and Design Method (SSADM)

## 92. DETECTION OF INFLUENTIAL OBSERVATIONS IN CANONICAL FACTOR ANALYSIS

ZENAIDA F. MATEO

*Department of Statistics*

*Central Luzon State University, Muñoz, 3120 Nueva Ecija*

Sensitivity analysis procedures have been previously studied by Tanaka and Odaka for detecting influential observations. Some of these analysis/procedures are the principal factor analysis, maximum likelihood factor and least squares factor analysis.

In the present study, it was shown that a similar method can also be developed in canonical factor analysis (CFA). The main objective here is to investigate the influence of a small change of data on the result of the analysis. One of the influence measures utilized to detect/assess influence observation is called Euclidean norm of  $\dot{A}^{(1)}$ . It is note mentioning that some techniques such as the usage of the Cholesky decomposition and its derivative are used to formulate the sensitivity analysis. First, the theoretical influence functions  $s(X; \dot{A})$  and  $s(X; LL)$  for the unique variance matrix  $\dot{A}$  and the common variance matrix  $LL$ , were derived and utilized in the formulation of theory.

The present method was applied to the Open/Closed book data (Mardia, Kent, Bibby, 1979). The data cover 88 students who took examinations in the five area subjects namely mechanics, vector, algebra, analysis, and statistics. The examinations of the five subjects were administered using a closed book and an open book method. A two-factor model is assumed and the canonical factor analysis was applied based on the correlation matrix.

The results showed that the two individuals No. 82 and 75 are the most influential among the 88 observations. It was observed that omission of these two observations is not small and influence appears mainly in the loading and communalities of the two subjects, that is in variable 1 (mechanics) and variable 2 (vector).

Considering the whole data set, the study revealed that there are two factors extracted namely: "Closed book test: and "Open book test". Omission of these two observations resulted to a vague structure, which suggest that the two individuals play important role in the analysis.

**Key words:** influential observations, canonical factor analysis, Euclidean norm, Cholesky decomposition, unique variance matrix, common variance matrix

### 93. DEVELOPMENT OF A CELLULAR AUTOMATA MODELING TOOL ON A CLUSTER COMPUTER

RAFAEL D. SALDAÑA and WILLIAM EMMANUEL S. YU  
*High Performance Computing and Networking Laboratory  
Ateneo de Manila University, Loyola Heights, 1108 Quezon City*

A cellular automaton (CA) is defined as a discrete dynamical system, where space, time, and the states of the system are discrete and have the following properties:

- (1) Space is represented by a regular lattice in one, two, or three dimensions.
- (2) Each site, or cell, in the CA lattice can be in one of a finite number of states.

Using the C programming language and the Local Area Multicomputer-Message Passing Interface (LAM-MPI) parallel computing environment, we developed a CA modeling and simulation tool on a cluster computer consisting of eight compute nodes.

The toolkit integrates four standard CA algorithms, namelyL (1) Game of Life, (2) Greenburg-Hastings, (3) Cyclic-Space, and (4) Hodgepodge Machine.

The developed modeling and simulation tool can be used to demonstrate the following complex phenomenal artificial life forms, neuron excitation, spread of diseases, and wave propagation in excitable media.

**Key words:** cellular automata, cluster computer, parallel computing, excitable media, modeling and simulation

## 94. A HYPOTHETICAL PERPETUAL MOTION MACHINE OF THE SECOND KIND

ARNOLD M. VIRAY  
Block 7, Lot 18 La Paz Homes  
Trece Martirez City, Cavite

A perpetual motion machine of the second kind is an impossibility, according to the second law of thermodynamics. The machine refers to a continuously-operating device that extracts heat from a reservoir at a particular temperature and then converts this heat completely into work. Its impossibility rests on the assumption that a heat-to-work conversion requires a temperature difference.

Any device for converting heat into work is called a heat engine, whose operation involves, typically, the following:

- 1) a high-temperature reservoir at absolute temperature  $T_1$  supplies heat to the engine
- 2) a portion of the inputted heat is converted by the engine into work
- 3) the remaining heat is exhausted to a low-temperature reservoir at absolute temperature  $T_2$ .

How efficiently the conversion takes place is a function of the temperatures of the two reservoirs:

$$e_{\max} = 1 - T_2/T_1$$

This equation, which defines the maximum thermal efficiency, affirms that assumption on which the second law depends; i.e., a heat-to-work conversion requires a temperature difference. Thus, if we are to harness the heat content, say, of the atmosphere at 300 K in order to operate a conventional heat engine, we must provide another reservoir at a sufficiently lower temperature.

Such a requirement, however, is bypassed in the following hypothetical heat engine-in essence, a multimicrogenerator system activated by spontaneous pressure fluctuations arising from the intrinsic random molecular motion of the gaseous substance.

For the derivation of this second-circumventing-technological-possibility, three principles are relied mainly upon: Brownian motion, electromagnetic induction and energy conservation.

**Key words:** hypothetical perpetual motion Machine

## 95. THE EFFECT OF USING PELLETIZED MEDIA ON $\alpha$ - AMYLASE PRODUCTION BY SOLID-STATE FERMENTATION IN AN AERATED PACKED-BED BIOREACTOR

APOLLO C. ARQUIZA<sup>1</sup> and WILFREDO I. JOSE<sup>2</sup>

<sup>1</sup>*Department of Chemical Engineering, College of Engineering and  
Agro-Industrial Technology  
University of the Philippines Los Baños, College, 4031 Laguna*

<sup>2</sup>*Department of Chemical Engineering, College of Engineering  
University of the Philippines Diliman, 1101 Quezon City*

Biotransformation processes, when compared to their chemical counterparts, offer the advantages of high selectivity, mild operating conditions, and the use of a wide variety of inexpensive raw materials (e.g. agricultural wastes). Most industrial fermentation use the submerged fermentation process (SmF) but another technique, solid state fermentation (SSF), is considered as a promising alternative for some biotransformation processes because of its advantages over SmF.

The study investigated the effect of using palletized media on the performance of an SSF system, particularly on an aerated packed-bed bioreactor. The SSF utilized *Aspergillus oryzae* grown on a rice bran-cassava starch medium (10:1 mass ratio) to produce  $\alpha$ -amylase. The palletized medium had an effective diameter of 5 mm compared to less than 0.833 mm for the unpelletized one. The column bioreactor used had a diameter of 100 mm and a bed height of 165 mm (total bed volume of 1.3 dm<sup>3</sup>). At an aeration rate of 1.20 vessel volume per minute (vvm) and 84 hours fermentation time, the palletized medium gave a yield of 589 dextrinizing unit (DUN)/(g dry medium) compared to 179 (DUN)/(g dry medium) for the unpelletized medium at the same conditions. Compared to that reported for SSF in static trays, the palletized medium gave 6.52 greater value. At 3.40 vvm aeration rate, the yield (palletized medium) was 611 DUN/ (g dry medium), which was 1.55 times that for the unpelletized medium and 6.76 times that for trays.

The effects of aeration rate and length of fermentation were further investigated for the palletized medium. The results show that the yield of  $\alpha$ -amylase did not vary significantly ( $\alpha = 5\%$ ) for aeration rates of 1.20, 2.06, 2.81, and 3.40 vvm. A fermentation time of 120 h produced an  $\alpha$ -amylase yield that was 60% greater than that for 84 h.

**Key words:** solid-state fermentation (SSF), packed-bed, bioreactor, palletized, *Aspergillus oryzae*, aeration,  $\alpha$ -amylase, enzyme, heat transfer, rice bran

## **96. PRODUCTION OF CRUDE INSECTICIDAL SUCROSE ESTERS FROM PALM KERNEL OIL**

REYNALDO L. ACDA and DESIREE G. CONDE

*Department of Chemical Engineering, College of Engineering and  
Agro-Industrial Technology  
University of the Philippines Los Baños, College, 4031 Laguna*

Crude insecticidal sucrose esters were produced from palm kernel oil through saponification, acidification, fatty acid chloride formation and acid chloride-sucrose reaction. The effect of varying the amount of concentrated HCl (2 ml, 4, ml, 6 ml, 8 ml, 10 ml, and 12 ml) per 10 g of palm kernel oil soap sample at 95°C on the fatty acid yield, the effect of increasing the amount of thionyl chloride (using 0.025 mol, 0.07 mol, 0.05 mol, 0.1 mol, and 0.125 mol) per 10 g fatty acid or 0.05 mole fatty acid (as lauric acid) on the acid chloride formation, the fatty acid (as lauric acid) on the acid chloride formation; and the efficacy of crude insecticidal sucrose esters on whitefly were determined.

The results showed that palm kernel oil saponified with 35° Be caustic soda (soap 1) yielded 16.84% free fatty acid and caustic potash (soap 2) with similar concentration in ethanol yielded 17.64% free fatty acid using 10 ml of concentrated HCl. Using various amount of thionyl chloride (1:2 fatty acid-thionyl chloride molar ratio) giving 11.2 g and 15.3 g fatty acid chloride from soap 1 and 2, respectively. Sucrose ester yield presented a high conversion of 72.91% and 76.32% based from the sucrose and acid chloride reaction.

Whitefly bioassay results showed that an average of 122 minutes, 100% mortality of whiteflies occurred. There was a significant difference between methanol, crude sucrose esters from soap 1 (ISE I) and crude sucrose esters from soap 2 (ISE II). No significant difference between ISE I and ISE ii as the results were subjected to a 5% level of significance ( $\alpha$ ).

**Key words:** palm kernel oil, insecticidal sucrose esters, whitefly bioassay

## **97. STUDY ON EFFECT OF FERMENTATION-CONDITIONS AND MODELING OF SUBMERGED BATCH PROCESS FOR CITRIC ACID PRODUCTION**

CHAY B. PHAM, RAQUEL B. MARQUEZ, and JOCELYN T. DE GUZMAN

*National Institute of Molecular Biology and Biotechnology (BIOTECH)  
University of the Philippines Los Baños, College, 4031 Laguna*

The demand of citric acid requirement in the country is met by importation. Citric acid is used in food, pharmaceutical, feed and medical industries. This study

was carried out to optimize the effect of initial ammonium and glucose concentrations and pH using multiple regression equation and to model the kinetics of submerged batch fermentation of citric acid production by *Aspergillus niger*.

Initial ammonium concentration effects on glucose, biomass and citric acid concentrations are shown by ANOVA ( $p > F = 0.01\%$ ). The highest citric acid concentration 84.10 g/l was obtained from 0.1 g/l initial ammonium concentration at 30°C, pH 3.5, 0.8 vvm aeration and 400 rpm agitation rate.

The fermentation kinetics related to growth model, production formation, substrate consumption were used to determine the kinetic parameters (i.  $q_m$ ,  $k$ ,  $C$ ,  $D$ ) using Leudeking-Piret equations. At the optimum fermentation conditions, the specific growth rate  $\mu$  for 1 g/l initial ammonium concentration was  $0.071 \text{ h}^{-1}$ . The non-growth related parameter,  $q_m$  (0.0095 g.product/g.biomass.h) was obtained at 1.0 g/l initial ammonium concentration indicating that product formation is growth related. Substrate consumption was also growth related since higher value of growth related parameter  $C$  (1.6558 g.substrate/g.biomass) was obtained as compared to the non-growth related parameter  $D$  (0.0458 g.substrate/g.biomass.h).

**Key words:** citric acid production, optimization of fermentation-conditions, modeling of submerged batch process

## 98. VISCOSITIES OF PURE AND BINARY MIXTURES OF METHYL LAURATE, METHYL MYRISTATE AND METHYL PALMITATE AT 30, 40, 50, 60, 70, 80, 90 °C

CARL D. SAQUING, APOLLO C. ARQUIZA, and JEFF AZUL

*Department of Chemical Engineering*

*College of Engineering and Agro-Industrial Technology*

*University of the Philippines Los Baños, College, 4031 Laguna*

The viscosity was measured for the pure, binary mixtures for the lauric, myristic and palmitic methyl esters (ME) and mixture for at least five MEs, at temperatures 30, 40, 50, 60, 70, 80, 90°C and a pressure of 1 atm using a capillary flow method equipped with a Ubbelohde viscometer. The data measured already are many (about 80 data points) and of exceptional quality, having relative standard deviations not exceeding 4.0% representing at least three trials for each data point.

Results showed that viscosity decreased with increasing temperature, but increased with increasing chain length. The measurements were correlated with Fulcher and Andrade equations for pure MEs, and Arrhenius and Nissan-Grunberg equations for binary mixtures. All the equations gave a very satisfactory fit to the viscosity of the pure and liquid mixtures studied. In each case, no percentage difference was greater than 4% between experimental and calculated results.

A generalized equation and a graph relating viscosity to the number of carbon atoms and temperature were developed. Such an equation and graph would be useful in predicting the viscosity of any methyl ester given the number of carbon atoms and temperature. Initial results manifest that very good prediction is achieved at higher temperatures, while more improvements are to be desired at lower temperatures. This may be due to the fact that non-idealities by virtue of stronger molecular interactions are more pronounced at lower temperatures. Further studies are being done to incorporate this in the model. The Grunberg-Nissan interaction energy constants are also reported, along with their analyses.

Finally, the viscosity of the methyl ester mixture produced from coconut oil was found to be closest to the binary mixture of 70% methyl laurate and 30% methyl myristate, hence can be a good approximation to the multicomponent mixture.

**Key words:** viscosity, Ubbelohde, viscometer, methyl esters, methyl laurate, methyl myristate, methyl palmitate, mathematical model, equipment design, generalized equation, carbon atom

## 99. THE EFFECTS OF DISSOLVED ACETATE SALTS ON THE VAPOR-LIQUID EQUILIBRIA OF THE ETHANOL-WATER MIXTURES

CARL D. SAQUING<sup>1</sup>, ALVIN I. REMOROZA<sup>1</sup>, APOLLO C. ARQUIZA<sup>1</sup>,  
and ELIZABETH BUGANTE<sup>2</sup>

<sup>1</sup>*Department of Chemical Engineering, College of Engineering and  
Agro-Industrial Technology  
University of the Philippines Los Baños, College, 4031 Laguna*

<sup>2</sup>*National Institute of Molecular Biology and Biotechnology  
University of the Philippines Los Baños, College, 4031 Laguna*

The effects of the potassium acetate and sodium acetate at 10% and 15% concentrations on the vapor-liquid equilibria (VLE) of the binary ethanol-water mixture were studied at atmospheric pressure using a modified Othmer still. Calibration using the ethanol-water mixture was done to check the reliability of the VLE apparatus on VLE determination. The results showed that the measured VLE data are close to published data.

The VLE data of the ternary mixtures of ethanol, water and salt were measured using the calibrated apparatus. Samples were collected at different temperatures ranging between the boiling points of pure ethanol and pure water, and were then analyzed by gas chromatography. Data showed that the addition of the two salts broke the ethanol-water azeotrope at all salt concentrations except for sodium

acetate at 10%. The addition of acetate salts increases the relative volatility of ethanol from 5 up to about 77, and the increase becomes higher as the salt concentration increases. Between the two salts, the increase in relative volatility is higher with potassium acetate in all concentrations. The more favorable effect of potassium acetate than sodium acetate may be explained by the stronger interaction of the former with water as indicated by its higher solubility in this solvent.

Moreover, activity coefficients ( $\bar{a}$ ) of the liquid samples were calculated from the experimental data and results manifested that the system with dissolved salts have higher  $\bar{a}$  than that of no-salt system. At one particular composition, the  $\bar{a}$  changed from 4.7 to 27.2. Thermodynamic consistency tests were performed on the data and were thermodynamically correlated using Wilson and NRTL activity coefficient models. Both models show good fit, but the Wilson model appears to be superior.

**Key words:** vapor-liquid equilibria (VLE), sodium acetate, potassium acetate, azeotrope, azeotropic distillation, extractive distillation, relative volatility, activity coefficient, entrainer, ethanol

## 100. UTILIZATION OF LOCAL RED CLAY FOR THE PRODUCTION OF TERRA COTTA BY SLIP CASTING

RAYMOND V. RIVERA VIRTUDAZO, CORONALYN PUGAT,  
ALMA PUYAOAN, BERNIE TAMAYO, CRISTETA ESQUIERDO,  
BEN EZRA APOLLO, and RODRIGO V. DEJETO  
*Department of Materials Science and Engineering,  
College of Engineering  
Mariano Marcos State University, Batac, 2906 Ilocos Norte*

Majority of local red-firing clays do not fit the slip casting method because red clays have a very complex behavior.

The study of casting properties of local red clays is deemed important to address the need of ceramic small company to find local red clay casting bodies with stable rheological properties, behavior and low production cost. The development of local red clay with identified fillers will provide a relative inexpensive raw material or finish product and create additional income to the community.

This research study focused on the development in casting behavior of the local red clay (Ilocos Norte) for Nanggyudan red clay, Macayepyep red clay and Baligat red clay. Slip casting method was used in order to evaluate the experimental



red clay (Nangguyudan, Macayepyep and Baligat red clay) for the development of Terra Cotta Product.

Result of the study show that Nangguyudan and Macayepyep red clays exhibit good casting properties based on the fluidity, physical properties and the experimental product that was produced in the research study. However, Baligat red clay can be costable at formulation 70:30 (clay – sand ratio) provided that it will follow specific procedure for casting methods.

**Key words:** fluidity, local red clays, slip casting, terra cotta

### **101. BINARY FORMULATION OF LOCAL WHITEWARE BODIES BY SLIP CASTING**

RAYMOND V. RIVERA VIRTUDAZO, CELIA BURGOS,  
MAYFLOR CACAO, and RODRIGO V. DEJETO

*Department of Materials Science and Engineering, College of Engineering  
Mariano Marcos State University, Batac, 2906 Ilocos Norte*

In the Ilocos region, the abundance of white clay explains the need to investigate, utilize and develop the raw material for earthenware products. White clays in Solsona have been studied using ternary formulation in which it passed the physical standard for earthenware bodies.

This study focused on the development of binary formulation of earthenware bodies utilizing only Solsona white clay and Ventura feldspar.

Wet screen method was used to homogenize the particle size and remove bigger size of organic materials present in the clay. Improvised radio magnet was also used in order to get or minimize iron content present in the local white clay.

Four (4) formulations were tested (90:10, 80:20, 75:25, and 70:30 of clay-feldspar ratio). The test specimen was fired at 850°C, 950°C and 1050°C. It was conducted to determine the physical (fire) properties and evaluate the formulated bodies for earthenware product.

Results of the study show that majority of 90:10 (clay:feldspar) formulation exhibits the highest results in linear shrinkage, change in weight, water absorption and apparent porosity at 850°C.

However, all the experimental binary formulations are possible to produce an earthenware product using the slip casting method based on the product results and data produced in the research study.

**Key words:** binary formulation, earthenware bodies, local feldspar, local white clay, slip casting

## **102. UTILIZATION OF LOCAL MATERIALS FOR THE MANUFACTURE OF FIRECLAY REFRACTORIES**

SAMUEL S. FRANCO

*Department of Materials Science and Engineering, College of Engineering  
Mariano Marcos State University, Batac, 2906 Ilocos Norte*

Fireclay is a basic refractory consisting of primarily hydrated alumino silicates with a silica ( $\text{SiO}_2$ ) content of up to 78% and an alumina ( $\text{Al}_2\text{O}_3$ ) and other minor constituents remaining not more than 38%. Fireclay materials vary widely in composition and in properties. Generally, firebricks based on kaolin show higher refractoriness and load resistance. Increase in the porosity of firebrick reduces the amount of spalling that occurs. Resistance to chemical attack is reduced with increasingly porosity. It is believed that a higher  $\text{Al}_2\text{O}_3$  content increases the resistance to attack by molten materials that contact the refractory materials.

Local clay materials and river sand were used in the formulation of the different refractory bodies. To increase the porosity and refractoriness of the refractories, local materials were used like saw dust, rice hull ash and coal. The proportions of the organic materials range from 2 to 10%. The refractories were fired at 1050°C, 1150°C and 1200°C. Slabbing was used in the making of refractories.

Local clay materials were found to be suitable for the manufacture of refractories for the construction of kilns of low firing ceramic products as well as for bakeries.

The porosity and the degree of refractoriness of the materials are directly proportional to the organic content. However, the strength of the refractories is inversely proportional to the organic materials added. The firing temperature of 1150°C was found to be the optimum temperature for firing refractories for local application.

## **103. EXTRACTION OF ESSENTIAL OIL FROM *Pogostemon cablin* BENTH (PATCHOULI) LEAVES USING SUPERCRITICAL CARBON DIOXIDE**

SUZETH V. NAVIDAD and ROBERTO M. MALALUAN

*Department of Chemical Engineering Technology  
Mindanao State University-Iligan Institute of Technology, 9200 Iligan City*

The supercritical carbon dioxide extraction of patchouli oil was studied using air-dried patchouli leaves as raw materials at temperatures 35°C and 40°C and pressures of 80, 100 and 120 atm. The percentage oil yield at 35°C at pressures

of 80, 100 and 120 atm averaged 4.86, 6.25 and 8.81%, respectively. At 40°C at the same pressures, the yields averaged 4.92, 7.15 and 8.93%, respectively. The conventional steam distillation process used by Pilipinas Kao Inc. yields only between 1.3 to 1.8% from air-dried samples of patchouli leaves.

Colors of the supercritical carbon dioxide extracts were yellow. The intensity of the color however, increased as temperature and pressure were increased. The extract obtained at 40°C and 100 atm was considered good since no waxy substances were obtained under said conditions.

The refractive index of the supercritical carbon dioxide extract at 40°C and 100 atm was 1.37192 and that from the steam distilled extract was 1.50840.

Gas chromatographic analyses were done for the different SC-CO<sub>2</sub> extracts and the extract from the steam distillation process. Chromatograms from SC-CO<sub>2</sub> extracts showed a few peaks while that of the steam distilled-extract showed many peaks. The presence of several peaks in the latter extract indicates the formation of other components due to thermal degradation.

The percentage oil yield at 40°C and 100 atm was 7.15%. This condition was chosen to be the best among other conditions because it was at this temperature and pressure that no waxy substances were observed.

The conditions of 40°C and 100 atm produced percent oil yield of 7.15% without any waxy substances. Thus, these conditions were chosen to be the best among the conditions tested.

#### **104. VOLTAMMETRIC DETERMINATION OF LEAD AND MERCURY USING CARBON PASTE ELECTRODES MODIFIED WITH WATER HYACINTH, *Eichhornia crassipes* (MART.) SOLMS.**

PRINCESS C. HERNANDEZ, JOSE H. SANTOS,  
MA. JAMELA R. REVILLEZA, and MAXIMA E. FLAVIER  
*Institute of Chemistry, College of Arts and Sciences  
University of the Philippines Los Baños, College, 4031 Laguna*

Water hyacinth, *Eichhornia crassipes* (Mart.) Solms., considered as one of the world's worst weeds, can cause reduction of water flow and restrictions in commercial fishing. However, these plants were reported to accumulate metal ions, a property explored in the present research to address monitoring of heavy metals. This study describes the use of a carbon paste electrode modified with the roots of *Eichhornia crassipes* (CPEMEC) for the determination of heavy metals such as lead and mercury by differential pulse anodic stripping voltammetry (DPASV). Water hyacinth obtained from Laguna de Bay was freeze dried to preserve the integrity of the metal-binding sites. The modifier was mixed with carbon powder in a 1:5 ratio and mineral oil added to form a paste. This was

packed inside a 2-mm diameter polyethylene tube and a copper rod was inserted to provide electric contact. The CPEMEC was used in the voltammetric measurements of Pb(II) and Hg(II) in aqueous solutions. For lead analysis, the sensitivity and detection limits were found to be  $6 \text{ iA}/10^{-6} \text{ M}$  and  $3.0 \times 10^{-9} \text{ M}$ , respectively. On the other hand, mercury (II) analysis gave a sensitivity of  $10 \text{ iA}/10^{-6} \text{ M}$  and a detection limit of  $1.2 \times 10^{-8} \text{ M}$ . Voltammetric response was optimized with respect to electrode composition, accumulation time, deposition time, pH, and deposition potential. DPASV using the modified electrode was used in the analysis of actual laboratory samples. The result obtained by DPASV was compared with standard AAS method and was found to be 30% lower. The ability of water hyacinth to accumulate metals was attributed to the ion-exchange properties of various functional groups present in the plant material. The ion exchange capacity of *Eichhornia crassipes* roots was also determined and found to be 2.72 G 0.21 meq/g using atomic absorption spectrometry (AAS).

**Key words:** anodic stripping, voltammetry, carbon paste electrodes, heavy metal analysis, chemically-modified electrodes, ion-exchange voltammetry

## 105. KINETIC AND PARAMETRIC STUDY ON ENZYMATIC AQUEOUS EXTRACTION PROCESS OF PILI KERNEL OIL (*Canarium ovatum* ENGL.)

CHAY B. PHAM<sup>1,2</sup>, REX B. DEMAPELIS<sup>2</sup>, and FIEL ETHEL A. MORADA<sup>2</sup>

<sup>1</sup>*National Institute of Molecular Biology and Biotechnology (BIOTECH)*

<sup>2</sup>*Department of Chemical Engineering, College of Engineering and  
Agro-Industrial Technology*

*University of the Philippines Los Baños, College, 4031 Laguna*

Pili nut is one of the most important oil seeds of commercial value in the Philippines. Pili oil was superior in quality as compared to coconut oil. This study was carried out to optimize the process conditions of the enzymatic extraction of pili kernel oil and to determine the quality of pili kernel oil from the enzymatic extraction process.

The effect of enzymes, pH, temperature, reaction time, agitation speed, substrate concentration and enzyme concentration on the oil yield was optimized in batch process in the stirred tank bioreactor equipped with controller and monitor systems. The oil yield was 93.4% as compared to the oil obtained by solvent extraction, at the extraction conditions of pH 7.0, 45°C, 300 rpm agitation speed, 1:8 (kernel:water, w/w) ratio and 4% enzyme concentration.

Results show that the reaction rate of oil extraction from pili kernel was greatly dependent on the enzyme concentration. At optimum process conditions, the reaction rates for both catalyzed and uncatalyzed extractions are: (a) for the

uncatalyzed reaction:  $r_s = 0.0546 C_s$  and (b) for the catalyzed reaction:  $r_s = 0.281 C_s C_E$ ; where  $C_s$  = amount of oil in the substrate;  $C_E$  = enzyme concentration.

**Key words:** Pili, kernel oil, enzymatic extraction process, kinetic and parametric study

## 106. A POLYPYRROLE-BASED pH SENSOR CHARACTERIZED BY FLOW INJECTION ANALYSIS

MILAGROS A. ABAYA-PEREZ<sup>1</sup> and CHRISTINA A. BINAG<sup>2</sup>

<sup>1</sup>Central Luzon State University, Maligaya, Muñoz, 3119 Nueva Ecija

<sup>2</sup>Research Center for the Natural Sciences and Graduate School  
University of Santo Tomas, España, 1008 Manila

A conducting Polypyrrole-based pH sensor by flow injection potentiometry was developed and characterized. The electroactivation parameters optimized for polymerization consisted of 0.1 M pyrrole monomer in 0.1 M phosphate buffer (pH 7.0), and bovine serum albumin (3.0 mg) as dopant. A current density of 9.02 mA cm<sup>-2</sup> was applied to the platinum wire (0.102 mm Ø) for a 5-minute galvanostatic deposition. The Polypyrrole coated-pH sensor was placed in a fabricated wal jet Perspex glass cell. Its potentiometric response against a Ag/AgCl reference electrode was monitored using universal buffer solutions at working pH range of 3-10. Optimization of flow injection variables such as nature, concentration, and pH of carrier solutions and the length of the manifold's line tubing were investigated.

The Polypyrrole-based pH transducer was characterized electrochemically and the feasibility of the sensing device under the established working conditions was evaluated. The pH sensor showed a sub Nernstian response ( $m = -31.8$  mV/pH), a good Pearson's correlation coefficient (linearity,  $r = -0.996$ ) and a highly reproducible response (RSD = 1.803%). The sensor showed low hysteresis ( $\Delta m = -3.8$  mV/pH) and minimal drift at pH 7 (RSD = 0.443%) and at pH 10 (RSD = 0.708%). The sensor is highly selective ( $k_{ij} > 10^{-7}$ ) in the presence of Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>, Ca<sup>2+</sup>, Ac<sup>-</sup>, and NO<sub>3</sub><sup>-</sup> ions. The sensor's lifetime for a period of two months revealed a 3-fold decrease in the sensitivity, from -28.6 mV/pH to -10.3 mV/pH.

**Key words:** Polypyrrole, pH sensor, conducting polymer, potentiometry, Nernstian

## 107. POTENTIOMETRIC IODIDE-SELECTIVE ELECTRODE BASED ON CONDUCTING POLYANILINE MEMBRANE

KAREN S. SANTIAGO<sup>1</sup> and CHRISTINA A. BINAG<sup>2</sup>

<sup>1</sup>*Chemistry Department, College of Science*

<sup>2</sup>*Graduate School*

*University of Santo Tomas, España, 1008 Manila*

Doping is necessary during the electrochemical oxidation of conducting polymers in order to achieve electroneutrality. This study involves the use of a dopant in fabricating an inorganic anion sensor, specifically the iodide-selective electrode (I-SE) based on polyaniline (Pan) film.

In devising the iodide sensor, electrochemical polymerization was carried out using the following optimized conditions: 1:1 mole ratio of aniline monomer and potassium iodide, 0.10 M potassium hydrogen phthalate buffer solution at pH 4, 30-minute polymerization time without stirring, platinum wire support and 9.34 mA cm<sup>-2</sup> current density.

The sensor showed a hyper-Nernstian response of -73.05 (m) and a linearity of 0.9855 (r<sup>2</sup>) at a concentration range of 1.96 x 10<sup>-5</sup> to 9.56 x 10<sup>-3</sup> M I<sup>-</sup>, and an average response time of 2.2 minutes. Through cyclic voltammetry, the growth of Pan onto a platinum disc was monitored which exhibited its oxidized form at X0.9 V. Its membrane has been likewise investigated via Scanning Electron Microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS) that showed the semi-fibrous and elemental compositions of Pan, respectively. The characteristics of the devised Pan-based potentiometric I-SE proved its wide applicability in industrial and biological purposes.

**Key words:** polyaniline, conducting polymer, potentiometric sensor, Nernstian, CV, SEM, XPS

## 108. PRODUCTION OF ACTIVATED CARBON FROM PILI (*Canarium ovatum* ENGL.) NUTSHELLS BY AMMONIUM CHLORIDE ACTIVATION

JOVITA L. MOVILLON, REX B. DEMAFELIS, SIXTO A. VALENCIA,  
MICHAEL ANGELO B. PROMETILA, and MADELAINE V. GOMEZ

*Chemical Engineering Department, College of Engineering and Agro-  
Industrial Technology  
University of the Philippines Los Baños, College, 4031 Laguna*

Present technology regarding the utilization of pili nut into activated carbon (AC) is yet to be determined and explored. Zinc chloride is commonly used as the activating agent but for this study, ammonium chloride was tested because it is readily available, inexpensive, and its low sublimation temperature of 330°C made further extraction of activating agent unnecessary. The main objective of the study was to produce activated carbon from pili nutshells by ammonium chloride ( $\text{NH}_4\text{Cl}$ ) activation.

Crushed and sieved nutshell (obtained from Sorsogon, Albay) was carbonized in pyrolyzer and activated in a muffle furnace. The activated carbon samples were subjected to direct activation and a two-step activation.

Results showed that the charcoal yield ranges from 20.9 to 30.4%, 31.8 to 40.6% and 30.3 to 34.6% for untreated, direct activation and two-step activation process, respectively. The highest and lowest yield occurred at temperature of 400°C and 800°C, respectively. The direct activation process provided a better yield compared to untreated and two-step activation process. However, the direct activation carbon gave higher moisture content and ash content compared to two-step activated carbon. In terms of fixed carbon, the untreated carbon has the lowest value (28.1%) while the two-step activated carbon (88.7%) has the highest value. The bulk density of untreated carbon, direct activated carbon, and two-step activated carbon are 0.546, 0.449, and 0.489 g/ml, respectively. The two-step activation at 800°C gave the highest iodine number of 305.9 mg/g but the value is still substandard compared to commercial carbon that ranges from 600 to 1100 mg/g Iodine Number. Further characterization and parametric studies regarding the production of activated carbon from ( $\text{NH}_4\text{Cl}$ ) activation are recommended.

**Key words:** activated carbon, Pili nutshells, chemical activation, ammonium chloride activation

## 109. CARBON DIOXIDE SENSOR BASED ON A pH SENSITIVE POLYPYRROLE

BERNARD JOHN V. TONGOL<sup>1</sup> and CHRISTINA A. BINAG<sup>2</sup>

<sup>1</sup>*Research Center for the Natural Sciences*

<sup>2</sup>*Graduate School*

*University of Santo Tomas, España, 1008 Manila*

The measurement of carbon dioxide is essential in biotechnology, in health care, and in beverage industry. The simplest device for detecting dissolved CO<sub>2</sub> is the Severinghaus electrode. However, the pH-glass electrode used in Severinghaus electrode is bulky and fragile.

In this study, a Severinghaus-type carbon dioxide sensor is fabricated using conducting Polypyrrole (PPy) as the pH sensing device. The PPy was polymerized galvanostatically ( $I = 1 \text{ mA}$ ) onto a Pt wire ( $0.17 \text{ cm}^2$ ) for 5 min in a solution containing 1.0 M pyrrole and 0.1 M NaHCO<sub>3</sub> solution. The PPy-pH sensor gave a sub-Nernstian response of  $-43.44 \text{ mV/pH}$  with a very good linearity of  $-0.999$  for three replicate measurements. For the fabrication of the CO<sub>2</sub> sensor, the PPy-pH sensor and the Ag/AgCl reference electrode are immersed in a mixture of 0.001 M NaHCO<sub>3</sub> and saturated KCl solutions. The sensor body is then covered with a gas permeable membrane. The sensor is sensitive to dissolved CO<sub>2</sub> gas from  $1 \times 10^{-2} \text{ M}$  to  $1 \times 10^{-5} \text{ M}$  NaHCO<sub>3</sub> solution. Further investigation is underway in view of optimizing the CO<sub>2</sub> sensor. A Pt disc which has a greater surface area than the Pt wire electrode has been employed, as well, for the electrodeposition of PPy. Surface morphology of the polymer-modified electrode has been studied using SEM while the elemental composition of the electrode surface has been analyzed through XPS and TOFSIMS.

**Key words:** carbon dioxide, carbon dioxide sensor, pH-sensitive, conducting Polypyrrole, SEM, XPS, TOFSIMS

## 110. POLY(3-METHYL THIOPHENE)-MODIFIED ELECTRODE FOR ELECTROCHEMICAL DETERMINATION OF DOPAMINE

REGINA AILEEN MAY V. VERGARA<sup>1</sup> and CHRISTINA A. BINAG<sup>2</sup>

<sup>1</sup>*Research Center for the Natural Sciences and*

<sup>2</sup>*Graduate School*

*University of Santo Tomas, España, 1008 Manila*

Dopamines occur naturally in our body. Dopamine is localized in certain regions of the central nervous system where it is an important neurotransmitter.



Detection of dopamine in the human body is of great importance to neuroscientist.

A poly(3-methylthiophene) modified (P3MTp) electrode offers substantial improvements in voltammetric sensitivity towards dopamine. Thin films of P3MTp have been electrochemically coated onto a platinum electrode and used for dopamine measurements. This P3MTp modified electrode enhances the oxidation peak current of dopamine while voltammetric response of ascorbic acid peak potential is greatly attenuated compared with that of a bare electrode. Surface morphology of the electrode has been analyzed with SEM while the elemental composition of the modified electrode surface has been studied using XPS analysis.

**Key words:** dopamine, poly(3-methyl thiophene), ascorbic acid, cyclic voltammetry, surface morphology

## 111. STATIC AND DYNAMIC HUGONIOTS OF $ZnSe_xS_{1-x}$ SINGLE CRYSTALS

SHIRLEY TIONG-PALISOC

*Physics Department, De La Salle University,  
2401 Taft Avenue, 1004 Manila*

The static phase transition points of ZnSe and  $ZnSe_xS_{1-x}$  (0.40 d" x d" 1) single crystals in the high pressure region are determined based on the transformation pressures of Bi I-II, Bi III-V and ZnS using the cubic anvil method where the pressure-induced variation of resistance is measured. The transition pressures of the samples vary linearly with the composition of ZnS in the  $ZnSe_xS_{1-x}$ . The shock compression curves of  $ZnSe_{0.85}S_{0.15}$  single crystals are also investigated. The pressure-particle velocity Hugoniot is found to agree with the corresponding Hugoniot of ZnS and ZnSe up to the phase transition point. The P-V isotherm of  $ZnSe_{0.85}S_{0.15}$  derived from the  $U_s - U_p$  Hugoniot is consistent with the calculated P-V curve based on Bridgman's static data of ZnS and ZnSe.

**Key words:** Hugoniot,  $ZnSe_xS_{1-x}$ , static, dynamic, high pressure, phase transition, cubic anvil, shock wave, Bridgman, semiconductor

## 112. HYDROTHERMAL SYNTHESIS (BY DIRECT DISSOLUTION AND VIA TRANSFORMATION OF LAYERED PRECURSOR) OF AN AKAGANEITE-TYPE IRON OXIDE OCTAHEDRAL MOLECULAR SIEVE

ELAINE NICOLAS-TOLENTINO and PAMELA ALFORNON  
*De La Salle University, 2401 Taft Avenue, 1004 Manila*

Iron oxide octahedral molecular sieve with akaganeite-type structure (2x2 tunnel), designated as FeO<sub>x</sub>-OMS (2x2) was successfully synthesized by hydrothermal method. The prepared FeO<sub>x</sub>-OMS (2x2) has high degree of purity based on X-ray powder diffraction (XRD) analysis and higher thermal stability than those of previously reported akaganeite-type materials. Thermal gravimetric analysis shows that the material is thermally stable up to 255°C in nitrogen atmosphere. At temperatures higher than this, the structure collapses and at 402°C, a new phase is formed which is hematite-magnetite based on its XRD pattern. The scanning electron microscopy (SEM) analysis reveals needle-like morphology which is a common characteristic feature of tunnel structures.

Synthesis of the akaganeite-type material via the transformation of a layered, lepidocrocite-type material, referred to as 1-FeO<sub>x</sub>-L2 to the tunnel structure is reported. This is the first successful conversion of a layered iron oxide as a precursor to a tunnel material. SEM micrographs further support this transformation as the plate-like morphology of 1-FeO<sub>x</sub>-L2 turned into needles. Thermal stability, however, of this material is much lower (195°C) than that prepared via direct dissolution using the hydrothermal method.

## 113. STRUCTURAL ANALYSIS OF COMMERCIALY IMPORTANT POLYSACCHARIDES FROM PHILIPPINE SEAWEEDS

JENNIFER T. AGUILAN, EDWARD T. CHAINANI, ARMANDO H. DE JESUS, MA. CRISTINA A. DANCEL, MILADY R. NIÑONUEVO, MARITES J. PASUELO, and FABIAN M. DAYRIT  
*National Chemistry Instrumentation Center and  
Department of Chemistry, School of Science and Engineering  
Ateneo de Manila University, Loyola Heights, 1108 Quezon City*

This paper aims to present studies on the structural analysis of commercially important polysaccharides such as *kappa* (*k*-) and *iota* (*i*-) carrageenan obtained from major sources of Philippine seaweeds such as *Kappaphycus alvarezii*, *K. cottonii*, *Kappaphycus* sp. "sacol" variety and *Eucheuma denticulatum*.

The polysaccharide content of fresh seaweeds was analyzed *in situ* using FT-IR microscope. Film samples of carrageenan extracts were also prepared from native and alkali modified extract and analyzed using the FT-IR spectrophotometer. Results obtained from both techniques were found to be comparable. The absorption peak observed at  $845\text{ cm}^{-1}$  was characteristic of the sulfate groups at C-4 position of the galactopyranosyl residue of the *k*-carrageenan extracts from all three *Kappapycus* species. On the other hand, absorption peaks observed at  $805\text{ cm}^{-1}$  and  $845\text{ cm}^{-1}$  correspond to the sulfate groups found at the C-4 position of the galactopyranosyl residue and at the C-2 position of the 3, 6-anhydrogalactopyranosyl residue from the *i*-carrageenan extracted from *E. denticulatum*.

One dimensional  $^1\text{H}$  and  $^{13}\text{C}$  NMR experiments were also performed on the native and alkali modified extracts obtained from the four seaweeds species studied. The anomeric signal due to C-1 of the 3, 6-anhydrogalactopyranose unit (*k*-A1) at 95.2 ppm is the major identifying feature of the *k*-carrageenan bearing seaweeds such as the three *Kappapycus* species studied. The anomeric signal due to C-1 of the 3, 6-anhydrogalactopyranose unit (*t*-A1) at 91.9 ppm is the major identifying feature of the *i*-carrageenan bearing seaweeds such as the *E. denticulatum* studied. Information on the presence of minor polysaccharide components detected from the  $^1\text{H}$  and  $^{13}\text{C}$  NMR were also reported.

The monosaccharide constituent analysis was performed by preparing alditol acetate derivatives by partial reductive hydrolysis of the carrageenan extracts. The glycosidic linkage was determined from partially methylated alditol acetate samples. All derivatized samples were analyzed using the GC-FID and GC-MS. Results show that a ratio of 43.2 (%):48.7(%) of 3, 6-anhydrogalactose: galactose content on the average were obtained from the three *Kappapycus* species while a ratio of 29.6(%) : 63.8(%) was obtained for *E. denticulatum*. This shows that major monosaccharide components are a galactose and a 3, 6-anhydrogalactose which are actually the sugar units which form the disaccharide repeating unit of carrageenan. Results from the methylation or linkage analysis show that for all three *Kappapycus* species the major components are 41.4% 1,4,5-tri-O-acetyl-2-mono-O-methyl-3,6-anhydrogalactitol and 48.6% 1,3,4,5-tetra-O-acetyl-2,6-di-O-methylgalactitol was obtained for *E. denticulatum*. The results show and confirm that the type of linkage is a 1  $\rightarrow$  3 linked galactopyranosyl residue and 1  $\rightarrow$  4 linked 3, 6-anhydrogalactopyranosyl residue.

#### 114. NON-ALKALOID COMPONENTS DETECTED IN TROPICAL YAM, *Dioscorea hispida* SCHLUSSEL

ALEXIE B. BANAAG<sup>1</sup>, HIROSHI HONDA<sup>2</sup>, SHIGERU MATSUYAMA<sup>3</sup>,  
and KAZUHIKO MATSUDA<sup>4</sup>

<sup>1</sup>*Department of Biological Sciences, College of Science and Mathematics  
Mindanao State University-Iligan Institute of Technology, 9200 Iligan City*

<sup>2</sup>*Laboratory and Applied Zoology*

<sup>3</sup>*Laboratory of Applied Biochemistry, Institute of Agriculture and Forestry  
University of Tsukuba, Tsukuba, Ibaraki*

<sup>4</sup>*Laboratory of Pesticide Chemistry, Kinki University*

Chemical analyses and structural elucidation of the naturally occurring active chemical components are very important for finding application, directly or as lead compounds or as new pest control agents.

Extracts of non-alkaloids were prepared by extracting the rhizomes of *D. hispida* with methanol, concentrated and re-extracted with ether. The ether extract was then concentrated by the same procedure above and subjected to open column chromatography eluted with different solvents. Mass spectra of non-alkaloid fractions were analyzed by 5890 Series II Plus Gas Chromatography and M-80B High Resolution mass spectrometer (in direct inlet mode).

Non-alkaloid chemicals from *Dioscorea hispida* which significantly controlled the activities of insect pest, *Plutella xylostella* L. (DBM) were identified. These activities affect insect's behavior as feeding deterrents, inhibitors of growth and development, and are also toxic against DBM Larvae.

These non-alkaloid chemicals were identified to be phthalate (compound 1), and unsaturated fatty acids (compounds 2 and 3).

**Key words:** *Dioscorea*, non-alkaloid, plant extracts, diamondback moth, unsaturated fatty acids

**115. MODE OF ACTION OF ISOQUINUCLIDINE ALKALOIDS  
FROM TROPICAL YAM, *Dioscorea hispida* SCHLUSSEL A  
GAINST RICE ARMYWORM, *Pseudaletia separata* LARVAE**

ALEXIE B. BANAAG

*Department of Biological Sciences*

*Mindanao State University-Iligan Institute of Technology, 9200 Iligan City*

Alkaloids have been studied intensively because of their medicinal importance and great diversity of structure and pharmacological activity.

This paper reports the effect of two alkaloids (dioscorine and dioscorine N-oxide) on the behavior of rice armyworm, *Pseudaletia separata*.

Several chemical components isolated from the rhizome of tropical yam, *Dioscorea hispida* have been found to have insecticidal and antifeedant activities to insect. Nothing is known about the mechanism of action of the isolated chemical of this tropical plant.

The behavioral effects of chemical components such as dioscorine and dioscorine N-oxide were examined against rice armyworm, *Pseudaletia separata*. The effects of the two alkaloids were compared to synthetic insecticides such as cartap, dichlorvos, and nicotine.

Isolated chemicals from *Dioscorea hispida* (dioscorine and dioscorine N-oxide) were found to have depressive effects against rice armyworm. These effects were similar to those of larvae treated with cartap. Hyperactive symptom was observed in dichlorvos and nicotine-treated larvae but not in larvae treated with the two alkaloids.

**Key words:** *Dioscorea*, armyworm, *Pseudaletia*, isoquinuclidine, alkaloids

**116. A NEW ALKALOID PREDICTED AS INTERMEDIATE IN  
THE BIOGENESIS OF THE *Pandanus* ALKALOIDS  
FROM *Pandanus amaryllifolius* Roxb.**

DAISY LOPEZ<sup>1</sup>, TOMOTAKE ICHIKAWA<sup>2</sup>, HIROMITSU TAKAYAMA<sup>2</sup>,  
MARIKO KITAJIMA<sup>2</sup>, NORIO AIMI<sup>2</sup>, and MARIBEL G. NONATO<sup>3</sup>

<sup>1</sup>*Graduate School, University of Santo Tomas, España, 1008 Manila*

<sup>2</sup>*Laboratory of Molecular Structure and Biological Functions  
Faculty of Pharmaceutical Sciences, Chiba University, Inage-ku,  
Chiba 603 Japan*

<sup>3</sup>*College of Science and Research Center for the Natural Sciences  
University of Santo Tomas, España, 1008 Manila*

Mature leaves of Marikina grown *Pandanus amaryllifolius* Roxb. collected quarterly throughout the year 1999 yield crude alkaloid fractions of similar TLC

profile. Alkaloids were detected in the dichloromethane, and n-butanol fractions obtained after extraction of the crude extract with solvents of different polarity (Hexane, dichloromethane and n-butanol). After a series of chromatographic purification, the dichloromethane yield five alkaloids.

A mid-polar alkaloid from the DCM fraction which was further purified by MPLC gave  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra identical to the secondary amine intermediate proposed in the biomimetic synthesis of Pandamarilactonine-A and -B [1]. These two alkaloids together with Pandamarilactone-1 [2] were also found in the dichloromethane fraction. Further 2-D NMR spectra of the secondary alkaloid confirmed its structure. This secondary amine is predicted biogenetically to be the possible intermediate of the reported *Pandanus* alkaloids.

### 117. THE IDENTIFICATION AND APPLICATION OF A YEAST LIPASE FOR THE BIOORGANIC SYNTHESIS OF (S+) -ARYL PROPIONIC ACID FROM RACEMIC PRECURSORS

ELLEANOR RIO C. ANDAYA, MILAGROS M. PERALTA,  
and MA. JAMELA R. REVILLEZA

*Institute of Chemistry, College of Arts and Sciences  
University of the Philippines Los Baños, College, 4031 Laguna*

The move to go in the direction of single isomer synthesis is gaining popularity since this will result in greater efficacy, faster relief and reduced toxicity. The present study aimed to identify an approach to synthesize single enantiomer chiral aryl propionic acid, ibuprofen, a model compound for non-steroidal anti-inflammatory drugs through a process known as enzymatic kinetic solution.

Four strains of *Candida*, the species first reported in the literature to exhibit enantiomeric selectivity in bioorganic reactions, were screened for hydrolase activities. An extracellular lipase from *Candida clausenii* exhibited the highest lipase activity of 312 U/mg and was chosen for the study. Production of the crude enzyme was optimized at pH 6.5 and 40°C. The enzyme was partially purified through DEAE anion exchange chromatography, eluting at 0.2 M NaCl. This resulted in an 11-fold increase in lipase specific activity when compared to the crude extract. SDS-PAGE analysis of the fraction indicated the presence of two protein bands at 59 and 67 kD, respectively. When used to catalyze hydrolysis of the synthetic ibuprofen buty ester, an apparent S(+) enantioselectivity, due to production of S(+) acid, was observed after HPLC analysis of the hydrolyses on a chiral column, S, S-Whelk-01 chiral column. With methyl ester as substance, no products resulted. The crude extract also showed preference for the S(+) enantiomer, the fast acting desired isomer, but peak intensity was low compared to the 0.2 M

fraction, emphasizing the importance of protein purification to select for the isoform that acts on the desired substrate.

**Key words:** lipase, yeast, enantioselectivity, enantiomer, chiral

## 118. TWO LECTINS FROM THE LEAVES OF MAHOGANY, *Swietenia macrophylla* KING: ISOLATION, PURIFICATION AND PARTIAL CHARACTERIZATION

ABIGAIL JOY D. RODELAS, MARIVIC S. LACSAMANA,  
and FLORINIA E. MERCA

*Institute of Chemistry, College of Arts and Sciences  
University of the Philippines Los Baños, College, 4031 Laguna*

Lectins are carbohydrate-binding proteins or glycoproteins of non-immune origin that can agglutinate cells and/or precipitate glycoconjugates. This study reports the presence of lectins in some Meliaceae species and the purification and partial characterization of two lectins from the leaves of *Swietenia macrophylla* King (large-leafed mahogany).

Crude leaf extracts of twelve Meliaceae species were screened for lectin activity using the hemagglutination assay. Eight of these species namely, *Azadirachia indica* (neem), *Dysoxylum cumingianum* (tara-tara), *Melia azedarach* (chinaberry/paraiso), *Melia dubia* (bagalunga), *Sandoricum koetjape* (santol), *Swietenia macrophylla* King (large-leafed mahogany), *Swietenia mahogany* (small-leafed mahogany) and *Toona calantas* (kalantas) gave positive results. The strongest lectin activity was observed in the crude leaf extract of *Swietenia macrophylla* King.

The lectins in the mature leaves of *Swietenia macrophylla* King were isolated by extraction with 0.02 M phosphate buffer containing 0.15 M NaCl, pH 7.2, and purified by sequential ammonium sulfate fractionation and gel permeation chromatography on Sephadex G-150.

The two purified lectins from the mature leaves of *Swietenia macrophylla* King namely, Lectin 1 and Lectin 2, were both non-blood type specific because they agglutinated all human blood types (A,B, O and AB). However, only Lectin 1 was able to agglutinate the calf, swine and carabao erythrocytes used in the study. Hapten inhibition assay using all four human blood types showed that the sugar specificity of Lectin 1 was directed towards several sugars such as L-(+)-arabinose, D-(+)-mannose, D-(+)-galactose,  $\alpha$ -L-rhamnose, methyl- $\alpha$ -D-mannopyranose, D-(+)-glucosamine, sucrose and  $\beta$ -D-(-)-fructose while the agglutination reaction of Lectin 2 was not inhibited by any of the sugars tested.

Both lectins were found to be glycoproteins containing 0.50% and 1.57% carbohydrate, respectively.

SDS-PAGE gave two protein bands for Lectin 1 with estimated molecular weights of 210 and 200 kD. For Lectin 2, only one protein band was observed with a molecular weight of approximately.

### 119. ISOLATION, PURIFICATION AND PARTIAL CHARACTERIZATION OF COCOSIN: THE COCONUT 11S GLOBULINS

ROBERTA N. GARCIA, EVELYN MAE TECSON MENDOZA,  
PERLA F. BALDIVIANO, and ANTONIO C. LAURENA  
*Institute of Plant Breeding, College of Agriculture  
University of the Philippines Los Baños, College, 4031 Laguna*

The major protein of the coconut endosperm is cocosin, one of a large class of seed storage proteins known as 11S globulins. This study aimed to isolate, purify and characterize the cocosin, an essential requirement in cloning and characterizing its gene.

Cocosin was isolated and purified by salt extraction (0.35M NaCl), Fast Protein Liquid Chromatography (FPLC)-gel filtration using HiLoad 26/60 Superdex 200™ column and FPLC-anion exchange chromatography with RESOURCE Mono Q™ column. The native molecular weight of cocosin was estimated to be 326000. Electrophoretic analysis revealed one set of 2 closely migrating bands at approximately 34,000 (acidic polypeptides) and another set of 2 bands at 24000 (basic polypeptides). Each set consisted of one darkly stained band and one lightly stained band. Preliminary N-terminal amino acid sequencing of the 34kD protein band gave the following sequence: SVRSVNEFRXE.

Cocosin was readily extracted by 0.35 mM NaCl. In the absence of  $\beta$  mercaptoethanol, the 55kD band representing the complexed subunit species was heavily stained indicating the presence of disulfide linkages in the molecule. All the bands tested positively for the presence of carbohydrate moieties using periodic acid-Schiff's reagent. Quanti-Scan analysis showed that cocosin comprised 80% of the total globulins.

**Key words:** coconut, 11S globulins, cocosin



## 120. PHYSICAL AND CHEMICAL CHARACTERIZATION OF THE ESTEROS IN QUIAPO, MANILA

JOYCE B. PERIA, MA. CARMELA B. SALAZAR,  
and BETTINA MARIA T. SILVERIO

*Environmental Science Program, School of Science and Engineering  
Ateneo de Manila University, Loyola Heights, 1108 Quezon City*

The *esteros* in Quiapo, Manila (i.e. *Esteros* de Quiapo, San Sebastian, and San Miguel) are tributaries of the Pasig, River, a lowland watercourse that is presently undergoing rehabilitation. Over the years, rapid urbanization in the area has contributed to the deterioration of water quality. In line with current efforts to rehabilitate the City of Manila, this study aimed to evaluate the quality of water in the *esteros* using the following physical and chemical parameters: temperature, dissolved oxygen (DO), pH, salinity, conductivity, turbidity, Biochemical Oxygen Demand (BOD), Nitrates concentration, and Total Phosphates concentration. The study also aimed to determine if an association exists between these parameters and the social activity in the area. Initial results showed high BOD and Total Phosphates concentration in all six test sites, exceeding the standards set by the Department of Environment and Natural Resources (DENR). However, Nitrates concentrations were well within DENR standards. The estero water quality has been adversely affected by the combined sewage of storm run-off and domestic waste in the area. Unfortunately, ongoing rehabilitation efforts for these waterways are inadequate. The results of the study will provide quantitative and qualitative data necessary for the establishment of an appropriate rehabilitation program for the *esteros*.

**Key words:** aquatic pollution, *esteros* in Quiapo, temperature, DO, salinity, conductivity, turbidity, BOD, nitrates, phosphates

