

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

## **1. CONSTRUCTION OF $r$ -REGULAR SINGULAR GRAPHS**

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A graph  $G$  is said to be *singular* if the adjacency matrix  $G$  is a singular matrix. For each integer  $r \geq 2$ , we determine here all values on  $n$  for which there exist connected  $r$ -regular singular graphs of order  $n$ . The constructions used in this paper make use of  $1$ -factors of the even complete graphs. It is known that when  $r = 2$ , the only connected  $2$ -regular singular graphs are the cycles whose number of vertices is divisible by 4. We prove here that if  $r \geq 4$  is even, there exist connected  $r$ -regular singular graphs of order  $n$  only for  $n \geq r + 2$ . When  $r \geq 3$  is odd, we show that connected  $r$ -regular singular graphs exist only when  $n$  is even and  $n \geq r + 3$ .

**Key words:** Graph, adjacency matrix, singular matrix,  $1$ -factor, connected graph, regular graph.

## **2. ON THE DIMENSION AND SPAN GRAPHS**

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The *dimension* of a graph  $G$ , denoted by  $\dim(G)$ , is the smallest nonnegative integer  $n$  for which the vertices of the graph can be represented objectively by points in the Euclidean  $n$ -space  $\mathbb{R}^n$  such that the distance between points corresponding to adjacent vertices is equal to 1. This paper gives bounds for  $\dim(G)$  as well as the sum  $\dim(G) + \dim(\bar{G})$ , where  $\bar{G}$  is the complement of  $G$ . The problem of inscribing a graph in a sphere in  $\mathbb{R}^n$  with as small a radius as possible is also

studied here. In particular, we show that every tree can be inscribed in a circle in  $\mathbb{R}^n$  with radius  $1/2 + \epsilon$ , for any  $\epsilon > 0$ . We show here how to construct a unit graph in  $\mathbb{R}^v$  out of a block *design* where  $v$  is the total number of points. The construction gives the well-known result that in a *1-design*, the number of blocks does not exceed the total number of points.

**Key words:** Euclidean space, distance, dimension, graph, complete graph, block design.

### 3. THE CHARACTERIZATION OF FINITE PSEUDOGROUPS OF SMALL ORDER\*

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A **pseudogroup** is a finite algebraic system compactly defined as: "*a not associative invertible loop*". The study of pseudogroup theory is relatively new, having been introduced only in 1981. Thus, in order to fully understand them, there is a need to determine the existence of a considerable number of non-isomorphic pseudogroups. This will enable the researchers in the field to have enough materials to use in order to study their properties and how they differ from other algebraic systems. In 1997, the author characterized all abelian pseudogroups of order 6. The results were presented in the 19th ASM of the NAST. The generation and analysis of all non-isomorphic pseudogroups of orders 5, 6, and 7 (abelian) have now been completed. In this paper these pseudogroups are presented and characterized according to the structural properties they possess, such as the number of subsystems, weak association properties satisfied, and the structural form. A total of 50 isomorphism classes were found and identified. Comparisons will be made regarding the properties of groups and pseudogroups, their similarities as well as their basic differences. All data were generated using computer software designed for the purpose.

**Key words:** Pseudogroups, isomorphism, structural properties, loops

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## 4. VARIABLE SELECTION IN FACTOR ANALYSIS REGRESSION AND ITS NUMERICAL APPLICATION

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Factors analysis (FA) regression is a statistical tool which can deal with the problem of linear prediction where the independent variables are subject to errors. It has been studied by several authors including Lawly and Maxwell (1973) and Browne (1988). Their works have made clear its basic properties. But, there still remain important problems such as sensitivity analysis and variable selection which have not been studied well. Therefore, our main target is to concentrate on these two problems. However, the part of variable selection procedure will be given more emphasis since the sensitivity analysis part had already been discussed in the paper of Mateo, Odaka, and Tanaka (1993).

In this paper, a backward elimination procedure is proposed for the selection of variables in FA regression. The squared correlation coefficient  $r^2(\beta)$  was used as a criterion to measure the adequacy of a regression model and for evaluating and comparing subset regression models. Some numerical investigations are presented to analyze the performance of the proposed variable selection procedure.

**Key words:** Backward procedure, factor analysis regression, ordinary analysis regression, ordinary least square regression, variable selection

## 5. DIBENZO-18-CROWN-ETHER IN SOL-GEL SILICON DIOXIDE MATRIX FOR METAL PRECONCENTRATION: I. SYNTHESIS AND CHARACTERIZATION

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Preconcentration is a common sample preparation technique in the analysis of trace metals. This study aims to develop a material composed of silicon dioxide

(SiO<sub>2</sub>) powder incorporated with dibenzo-18-crown-6 (DB18C6) which will be used to trap and preconcentrate trace metals in aqueous solutions. The SiO<sub>2</sub>-DB18C6 was synthesized using the sol-gel method with tetraethylorthosilicate (TEOS) as silicon precursor. The effects of catalyst used, pH, and solvent on the resulting products were determined. The stability of the silicon dioxide-dibenzo-18-crown-6 ether (SiO<sub>2</sub>-DB18C6) in acidic conditions was also investigated. SiO<sub>2</sub>, and SiO<sub>2</sub>-DB18C6 products were characterized using Fourier Transform Infrared (FTIR) spectroscopy, thermal gravimetric analysis/differential thermal analysis (TGA/DTA), scanning electron microscopy (SEM), and energy dispersive x-ray spectroscopy (EDX). Solid powder products were formed using ammonia as catalyst, while gelatinous films were formed using nitric acid as catalyst. The use of ethanol as solvent resulted in fastest drying compared to butanol and methanol, while it also showed the best ability to dissolve DB18C6. Infrared spectroscopy showed the characteristic peaks for SiO<sub>2</sub> and DB18C6. Similar spectra for both the SiO<sub>2</sub>-DB18C6 and acid-treated SiO<sub>2</sub>-DB18C6, indicated that no changes in bonding had occurred during acid treatment. SEM analysis of SiO<sub>2</sub>, SiO<sub>2</sub>-DB18C6, and acid-treated SiO<sub>2</sub>-DB18C6 showed that all products had uniform spherical particles with diameters ~0.4 μm. Thermal analysis indicated no major difference between the acid-treated sample and the untreated sample that suggests no major change in composition occurred during acid treatment. However, DB18C6 degraded at ~350°C and therefore, the SiO<sub>2</sub>-DB18C6 material can only be heat treated to remove trapped water at temperatures less than 350°C. The thermal profiles also showed that the SiO<sub>2</sub> matrix is also stable up to ~950°C. EDX results confirmed that silicon is the major component (~95% atomic composition).

**Key words:** Silicon dioxide, sol-gel, crown ether, trace metals, preconcentration, infrared spectroscopy, FTIR, TGA, DTA, SEM, EDX

## 6. SYNTHESIS OF LIQUID CRYSTALLINE SILICONES WITH CYANOBIPHENYL AND CHOLESTERYL PENDANT GROUPS

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Cholesteric polymers are of special interest to materials scientists and technologists because of their unique property of combined thermo-electro-optical sensitivity and mechanical property. In the synthesis of liquid crystalline silicones, the cyanobiphenyl is introduced as a side group to enhance the electro-optical property. The cholesteryl moiety as another side group is expected to enhance the



cholesteric nature, hence the possible thermo-optical property of the resulting polymers. To prepare the polymers, vinylic monomers containing the cyanobiphenyl group (4-( $\omega$ )-hexenoxy-4'-cyanobiphenyl) and cholesteryl moiety (cholesteryl 4-propenoxy-4'-benzoate) were synthesized, and were reacted with cyclic polysiloxane using the Speier's catalyst. The cyanobiphenyl-containing monomer was found to be nematic at a temperature range of 35.37°C to 52.66°C, whereas the cholesteryl-containing vinyl was found to be cholesteric from 106.97°C to 118.42°C. The synthesis and properties of the monomers and the resulting side-chain polymers will be presented.

**Key words:** Cholesteric, cyclosiloxane, cyanobiphenyl, liquid crystalline, nematic, polymers, silicone, Speier's catalyst, vinylic monomers, thermo-electro-optical

## 7. ARSENIC SPECIATION BY HYDRIDE GENERATION-ATOMIC ABSORPTION SPECTROMETRY COUPLES WITH A CRYOGENIC TRAP

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Hydride generation-atomic absorption spectrometry (HG-AAS) combined with a cryogenic trap was utilized in arsenic speciation. The set-up of the HG-AAS system consists of a peristaltic pump, PE 3100 atomic absorption spectrometer, 2 Variac transformers, and a strip chart recorder. Mixed solutions of inorganic arsenic (As III), monomethyl arsenic acid (MMAA), and dimethyl arsenic acid (DMAA) were converted to their corresponding volatile hydrides and the generated arsines trapped and separated according to their volatility: inorganic arsine first, then analysis of the different arsenic species. Linear responses were obtained in the nanogram levels. The technique was applied to arsenic speciation in some seawater and seaweed samples. The seawater samples contained an average of 1.5 ng/mL inorganic As. The seaweed sample analyzed contained inorganic arsenic species and DMAA totaling 0.5  $\mu$ g total As/g of seaweed.

**Key words:** Arsenic, atomic absorption, spectrometry, speciation, hydride generation, seawater

## 8. CALORIMETRY: ENTHALPIES AND ENTROPIES OF SOME METAL-CYANIDE COMPLEXES BY THERMOMETRIC TITRATION

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Thermodynamic modelling provides a method for predicting the chemical behavior of the complicated processes in the hydrometallurgical extraction of gold but is critically dependent on the availability of reliable data. Such thermodynamic data are limited or not available. Enthalpy changes associated with the complexation of some metals with cyanide were determined by titration calorimetry using an isoperibol (constant temperature environment) calorimeter. These calorimetric measurements were done in both aqueous NaCl and NaClO<sub>4</sub> media at an ionic strength of 1M.

The  $\Delta H$  values show slight to no dependency on the medium. Other thermodynamic properties are calculated from these  $\Delta H$  values with available stability constant or  $\Delta S$  values. These data are very important in the cyanide processes involving high ionic strength solutions.

**Key words:** Calorimetry, titration calorimetry, isoperibol, enthalpies, entropies, cyanides, cyanide complexes, metal cyanides, thermodynamic data, hydrometallurgical solutions, gold extraction

## 9. POTENTIOMETRIC pH-SENSOR BASED ON ELECTROPOLYMERIZED POLY (*o*-PHENYLENEDIAMINE)

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A novel potentiometric pH-sensor device was fabricated using galvanostatic electrochemical polymerization of poly (*o*-phenylenediamine) (PoPD) onto a Pt wire from a suitable buffer solution containing the doubly crystallized *o*-phenylenediamine and the dopant bovine serum albumin (BSA). Electrochemical polymerization

parameters of the sensor were optimized against Ag/AgCl electrode using buffer solutions of pH 3 to 10. The polymer-coated pH-sensor exhibited a high sensitivity with nearly Nernstian response and a slope of  $-47.5$  mV/pH, a good linearity ( $r = -0.991$ ), a reasonable response time (8 min at pH 3-10), a favorable repeatability at three (3) replicate measurements (RSD = 6% at pH 3-8), and a very high reproductibility (RSD < 3%) at 11 replicate and alternate measurements of pH 3 and 10 for a period of <2 h. This yellow-brown P $\alpha$ PD polymer coated Pt wire is a promising pH transducer for the analysis of pH changes in biological reactions acting as biosensor.

**Key words:** pH, sensor, poly(*o*-phenylenediamine), potentiometric, transducer, bovine serum albumin, polymer, electropolymerization, biosensor, Nernstian response

## 10. DESIGN OF A MICROCOLORIMETRIC ENZYME ASSAY FOR SCREENING OF RADIOPROTECTORS USING THE ORIENTAL FRUIT FLY *Bactrocera philippinensis* MODEL

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Loss of function and expression of a 109 kDa protein is observed in the Oriental fruit fly, *Bactrocera philippinensis*, upon exposure to a  $\gamma$ -radiation dose of 100 Gy. Found to possess tyrosinase activity, this marker enzyme is particularly important during quarantine treatment of export fruits. A semi-automated radioprotector screening assay for anti-cancer drug development at PNRI has been developed and optimized. Larvae of *B. philippinensis* are subjected to relatively high and low doses of standard radioprotectors (*l*-glutathione (GSH), *tert*-butylated hydroxyanisole (BHA), garlic bulb extracts), temperature treatments (37°C and 42°C), and relatively high and low radiation doses (10 and 40 Gy) following a 2-factorial design. Using mushroom tyrosinase as standard and 605 nm as reference wavelength, optimum precision, sensitivity and curve linearity are achieved at the 405 nm window within a 60-minute reaction time with 2-methyl DOPA yielding dopachrome. Significant radioprotection and tyrosinase activity are observed. Results showed that GSH exhibited the best radioprotection with an emergence rate of

100% (GSH<sub>h</sub> 42°10). Consequently, GSH<sub>h</sub> exhibited a high dopachrome level next to garlic<sub>h</sub>. Garlic approximates the performance of GSH and BHA, but the fact that dopachrome levels of garlic<sub>h</sub> are exceeding high could be correlated with the relatively lower emergence rates observed. A dopachrome level of 0.45-0.05 µg/ml exhibits the optimal radioprotection. Other radioprotectors will be screened in the future using this assay in search of potent and less toxic radioprotectors that could decrease radiation-induced morbidities and improve therapeutic gains in patients undergoing therapy.

**Key words:** Radioprotector, radiotherapy, *Bactrocera philippinensis*, anti-cancer drugs, radiation biology, natural products, cancer management, dopachrome, fruit fly, tyrosinase

## 11. CHARACTERIZATION OF FIBER, PULP, AND PAPER FROM TOBACCO STALK AND THEIR SUITABILITY FOR HANDMADE PAPER PRODUCTION

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Fiber, pulp, and paper derived from tobacco stalks were characterized in terms of their chemical and physical properties, such as total pulp yield, fiber dimensions, holocellulose and lignin contents, and paper strength properties. Conventional handmade paper making and paper products conversion were then done to establish the technical and economic feasibility of paper production from tobacco stalks.

Results showed that the pulp yield obtained from soda-pulp tobacco stalk was 64.89%. This is higher than those of rice straw, cogon grass, banana, and pineapple fibers, and comparable to abaca fiber, the most commonly used fiber for handmade paper. The average fiber length was 0.72 mm, which is within the moderately short fiber category.

The holocellulose content of tobacco pulp is comparable to that of jute.

Tobacco paper sheets made of pulp beaten for 15 minutes in a Valley beater are comparable to paper mulberry, maguey, and salago sheets in terms of tensile index, tear index, and burst index, respectively.

Practical handmade paper production also showed that even at higher charge of NaOH (15%) and at longer cooking time, the cooked fiber still retained its relative hardness and did not defibrillate readily like mulberry, cogon, and other fibers.

It was shown that with slight modification of some processes, e.g., pulping and beating, it is technically feasible to produce handmade paper from tobacco stalks. At current prices of handmade paper products, the profitability is assured and even surpasses the net income derived from the main crop.

**Key words:** Tobacco stalk, pulp, fiber, handmade paper, pulp yield, fiber length, holocellulose, tensile index, tear index, burst index

## 12. ANTIGENOTOXICITY STUDIES ON SPINASTEROL, AN ISOLATE FROM *Cucurbita maxima* FLOWERS

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Spinasterol was isolated from squash flowers by solvent partitioning and repeated vacuum liquid chromatography using a Micronucleus Test-directed scheme. At a dosage of 100 mg/kg mouse, spinasterol is antigenotoxic as it decreased the mutagenicity of tetracycline, a known mutagen, by 64.7% ( $\alpha=0.001$ ) using the micronucleus test, an in vivo method.

Spinasterol was then tested for its antitumorigenic and antiteratogenic potentials. The antitumorigenic activity was monitored using the mouse skin tumor assay. There was a 90% tumor incidence for the positive control group (DMBA + croton oil + acetone). At a concentration of 15.0  $\mu\text{g}/0.2$  mL acetone, spinasterol decreased the incidence of skin tumors by 55.6% when applied immediately after croton oil. It is not a co-carcinogen nor a co-tumor promoter as there was no increase in the incidence of skin tumors after spinasterol application. Hence, spinasterol showed antitumorigenic potential. Moreover, spinasterol was able to counteract the teratogenic effect of tetracycline as there was a significant decrease in the number of females with resorptions and a decrease in the number of dead implantations.

**Key words:** Squash flower, spinasterol, antimutagen, antiteratogenic, antitumorigenic, micronucleus test, dominant lethal skin, mouse skin tumor assay



### 13. MINIMIZING EMISSION OF CARBON DIOXIDE IN COCONUT PROCESSING

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About 90% of the world's coconut production is made into copra. There are 2-3 million smoke kilns which are used by the coconut farmers for making copra. It is estimated that these kilns emit carbon dioxide from 247 to 366 g of carbon per kg of copra produced. From the world copra production of 10 t, the total carbon released in copra making range is 2-3 Tg (teragram =  $10^{12}$  grams) or 2-3 t of carbon per year. To minimize carbon dioxide emission in copra making, kilns with better combustion characteristics and heat utilization efficiencies must be used.

One of the more promising alternative dryers is a direct-fired, natural draft dryer known as the Los Baños (Lozada) Dryer. Developed at the University of the Philippines Los Baños, the dryer consists of a simple burner, a heat distributor, and a drying bin. The burner combusts, coconut shell, corn cob, and wood pieces with extremely high efficiency, thus minimizing fuel consumption and dramatically reducing the release of airborne pollutants. The resulting copra is practically smoke-free. Tests have shown that carbon dioxide emissions from the Los Baños (Lozada) Dryer are about half of that released by the traditional smoke kilns. Furthermore, the dryer emits lower concentration of CO (50 ppm vs 2000-3000 ppm), of NO<sub>x</sub> (5 ppm vs 400 ppm), and SO<sub>x</sub> (5 ppm vs 400 ppm). When used widely, significant reductions in the emissions of greenhouse and acid rain gases from biomass combustion will be attained. (About 500 units of the Los Baños (Lozada) Dryer are now in use in the Philippines and Papua New Guinea).

**Key words:** Greenhouse gases, drying technology, copra making

### 14. RECYCLING OF DISTILLERY SLOPS FOR ETHANOL AND ACETIC ACID FERMENTATION

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Laboratory scale experiments of slops recycling on ethyl alcohol fermentation and acetic acid production were conducted. Back slopping was carried out

using a 25% slops solution for each cycle. The effect of the number of recycles on the fermentation efficiency was investigated.

Statistical analysis of data indicated that there was no significant difference in the fermentation efficiencies obtained for the five recycles, which means that the number of recycles did not adversely affect the fermentation efficiency.

The use of back-slopping was able to cut the wastewater generation by 18.42%. It therefore reduced the water consumption in the distillery by approximately the same quantity. The unrecycled slops were then used in the production of acetic acid.

The production of acetic acid was done using the standard method for acetic acid fermentation. An efficiency of 13.04% was obtained for the second set-up, 10.47 for trial A, 9.97% for trial B, and 3.03 for trial I. At the end of the fermentation, a total acetic acid content of 9.55 g, 9.37 g, 10.50 g, and 1.25 g for trials A, B, control, and I, respectively. These values are low compared to the commercial vinegar which has 40 g acetic acid for every liter. The low efficiencies and acid content were attributed to the absence of aeration during fermentation.

The use of back-slopping already resulted in a commendable reduction in wastewater generation, but the conversion of the excess slops to acetic acid, with the necessary refinements applied, will guarantee an almost zero wastewater generation. The recycling of slops using the said methods is therefore an effective and productive way of treating distillery wastewater.

**Key words:** Distillery slops, recycling, ethyl alcohol, acetic acid, fermentation

## 15. PRODUCTION OF ACONITIC ACID FROM MUSCUVADO MASSECUITE

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Aconitic acid is a useful compound in the preparation of plasticizers, in organic synthesis, and as a flavoring agent. Effective detergents can be prepared by the reaction of esters of aconitic acid with sodium bisulfite. Aconitic acid commanded a price of \$21.86 per 250 mg as of 1997.

Aconitic acid is the most abundant constituent acid of cane. Massecuite, an intermediate product of cane sugar manufacture, and final molasses, a by-product after centrifugation, contain aconitic acid in varying amounts depending on the location of sugarcane production. Some reports showed that aconitic acid is about 1-6% by weight of molasses. It is assumed that "muscuvado massecuite" contains

more aconitic acid, since in this process the sugar crystals are still intact in the mother liquor, and do not undergo centrifugation.

Aconitic acid crystals of purity 99.57% by mass, 3.2 g/100 mL solubility at 15°C, and melting at 194°C, were recovered from "muscuvado masecuite" which contained about 1.049% aconitic acid, giving an average of about 92% recovery by the ion exchange method using a weak base exchanger (polyamine), Amberlite IRA-95. Further purification treatments involved the use of 10% sulfuric acid, bentonite, and Dowex 50 W cation. It was observed that temperature had no significant effect on the yield of dried and pure aconitic acid. Based on the results, adsorption was optimum at 27°C and pH 5.58.

**Key words:** Aconitic acid, muscuvado masecuite, ion-exchange

## 16. DESIGN, FABRICATION, AND PRELIMINARY TESTING OF A BENCH-SCALE SPINNING BAND COLUMN FOR THE DEODORIZATION OF COCONUT OIL

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A spinning-band column was designed, fabricated, and tested for the deodorization of coconut oil. The helical spinning band was made of stainless steel perforated mesh that was spot-welded around a stainless steel shaft. A variable electric motor was connected to the shaft. The whole process is steam distillation. The coconut oil was scraped to the wall as the steam was introduced into the system.

The equipment was tested at 70° and 100°C and with flowrates at 1000, 750, and 500 mL/h. These conditions were evaluated by determining the %FFA, by spectrophotometric analysis and olfactory evaluation. The best operating condition was at 100°C and a flowrate of 500 mL/h. The %FFA was decreased from 0.2943 to 0.2400, and the highest % transmittance and the lowest color units were obtained.

It was found out that the higher the temperature, the shorter is the deodorization time and the longer the time of contact between steam and fat, the more efficient is the deodorization.

**Key words:** Spinning band, deodorization, coconut oil, decolorization

## 17. ELEVATED PERFORATED SOLAR DRIER

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Drying is one of the problems associated with crop production. Substantial portions of agricultural products are lost due to improper drying.

An inexpensive elevated "tray type" perforated platform solar dryer was designed and developed using a wooden frame with a screen mesh bottom. The wire mesh is used to hold the grain. The system of operation is simple. The tray containing the grain is placed in the platform at a depth of 5 cm. The elevation from the ground can be at 30, 45, 60, or 75 cm. It can be placed even in uneven surfaces and above grasses when conventional floor drying is not possible.

The dryer is effective even when solar radiation is low because the dry air is allowed to pass above, below, and through the grain bed. This is in contrast to open sun drying over the pavement wherein the air is passed only on the surface of the grain bed. The dryer is better than open sun drying over pavement or with the use of net or canvas. It can reduce the drying time by 10% and the milling recovery by 5%. The drying time of cracked and fermented grains can also be reduced with the use of the dryer.

The cost of the elevated platform dryer is comparable to that of the canvas or the plastic mesh dryer. It can be constructed by the farmer using basic tools like the triangle, cross-cut saw, and hammer. The dryer is portable and can be easily dismantled for safe keeping when not in use. It can also be used to dry other agricultural and fishery commodities.

**Key words:** Dryer, drying, palay, solar, milling, fermented grains, cracked grains

