



PACCON

PURE AND APPLIED CHEMISTRY
INTERNATIONAL CONFERENCE

2016



PROCEEDINGS

'THAILAND: One Hundred Years of
Advancement in Chemistry' **100**
Years

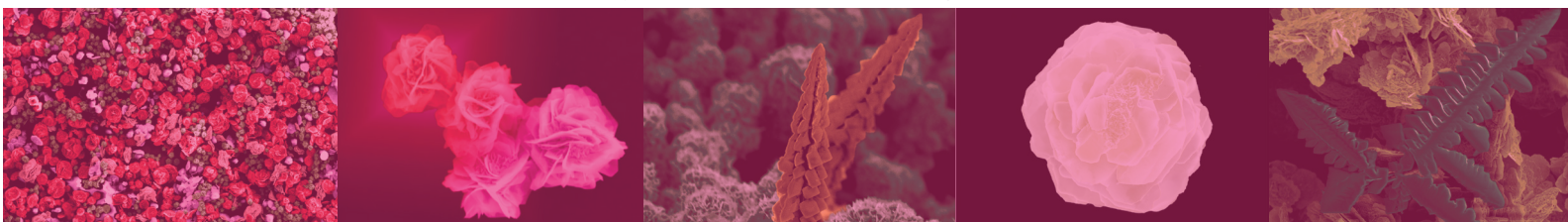
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กลุ่ม ปตท.คงสภานะ DJSI Member 2015

ในกลุ่มอุตสาหกรรมน้ำมันและก๊าซ (OIX) และ กลุ่มธุรกิจเคมีภัณฑ์อย่างต่อเนื่อง สะท้อนศักยภาพการดำเนินธุรกิจที่โปร่งใส มีจรรยาบรรณ มุ่งเน้นการมีส่วนร่วมของผู้มีส่วนได้ส่วนเสีย ควบคู่ดูแลสังคม สิ่งแวดล้อม เพื่อเสริมสร้างความแข็งแกร่งในการเติบโตอย่างยั่งยืนของประเทศ

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Proceedings

The Pure and Applied Chemistry International Conference 2016 (PACCON2016)

**“THAILAND: One Hundred Years of Advancement in
Chemistry”**

February 9 –11, 2016

at

**Bangkok International Trade and Exhibition Centre (BITEC)
Bangkok, Thailand**

Organized by

**The Chemical Society of Thailand under the
Patronage of Professor Dr. HRH Princess Chulabhorn**

In association with

**Department of Chemistry, Faculty of Science
Chulalongkorn University**



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Update/correction note

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Welcome Message from the President of Chemical Society of Thailand:

On behalf of the Chemical Society of Thailand (CST), it is my honor to invite all the distinguished delegates to the Pure and Applied Chemistry International Conference 2016 or PACCON2016. The coming PACCON2016 is held in conjunction with Department of Chemistry, Faculty of Science, Chulalongkorn University. It is also a great occasion for celebrating 100 years anniversary of Chulalongkorn University. As the President of the Chemical Society, I would like to express my sincere gratitude to the Chairman of the Chemistry Department, the Dean of the Faculty of Science, and the President of Chulalongkorn University for jointly hosting the international conference, PACCON2016.

Since the founding of the Chemical Society of Thailand in 1980, the first PACCON has been launched in 2008 and now the conference has brought together thousands of participants and invited speakers across Asia and the world to participating, disseminating, and sharing knowledge of recent advancement in chemistry and related areas. In addition to the main conference, we have also organized several important symposia as showcases of how the chemistry innovation progress in the past 100 years under the theme, "Thailand: One Hundred Years of Advancement in Chemistry".

As always, the conference will provide oral and poster presentations of pure and applied chemistry led by world well-known chemists who are experts in the areas. Moreover, we also provide a special session for teachers who are experts in teaching chemistry in school nationwide for acquainting them with international atmosphere. This is another activity of CST to promote education in chemistry at school level with the aim to increase public understanding of how importance of chemistry in improving their standard of living.

As the President of CST, I am particularly pleased to invite you all to join us for the PACCON2016 to be held in Bangkok, Thailand during February 9 – 11, 2016. This year's conference is a great opportunity to join with Chulalongkorn University to celebrate its 100 years anniversary. I wish all of the participants fruitful deliberations and believe that all of you will enjoy the sharing and exchanging of your expertise between thousands of expected delegates from different parts of the world. Other conference offerings to look forward to are the warm social activities, cultural exchanges, and lasting friendships that await all the distinguished delegates as they step into one of the great city, Bangkok, Thailand.

Associate Professor Dr. Surin Laosooksathit
President, the Chemical Society of Thailand



Welcome Message

Welcome Message



Welcome Message from the President of Chulalongkorn University:

Excellencies,
Distinguished Guests,
Ladies and Gentlemen,

Welcome to the vibrant city of Bangkok where the Pure and Applied Chemistry International Conference 2016 (PACCON2016) will be held during February 9 – 11, 2016. Chulalongkorn University proudly host the event as part of a commemoration on our centennial celebration on the establishment of the university where chemistry teaching was first offered in Thailand, and moreover, as we had initiated and co-hosted the very first PACCON back in 2002.

As Thailand's first institution of higher education founded nearly a century ago, the university produces highest quality graduates with a high level of knowledge and skills in the arts and sciences that they can use to contribute to society. Chulalongkorn University has been committed to ongoing development in programs, human resources, facilities and services. With the cooperation of alumni, we have been building an intellectual community devoted to serving Thai society and the nation. We are determined to graduate not just the best qualified but persons of integrity under the credo, "The Pride of Chula is in Serving the Public".

Therefore, I am sure that the PACCON2016 will be an excellent ground to express the advancement of chemistry in the past 100 years; to learn frontier pure and applied chemistry from all regions; to share new findings in modern areas of chemistry and other disciplines in academia and industries; to cherish collaborations and friendship among researchers of all races, ages, and disciplines which would ultimately pave the way to an even more advanced knowledge in the years to come.

I would like to extend my deepest gratitude to the keynote speaker, plenary speakers, invited speakers, those who have contributed their findings, and all the participants here at the conference. Moreover, I would like to express my sincere appreciation to our sponsors for making this conference financially possible. Finally, I truly thank the Chemical Society of Thailand (CST) under the Patronage of Professor Dr. Her Royal Highness Princess Chulabhorn, all the reviewers, organizing committee members, staff, and students who have tirelessly devoted their valuable time to make PACCON2016 one of the most memorable conferences of all time.

Professor Pirom Kamolratanakul, M.D.
President



Welcome Message from the Dean of Faculty of Science, Chulalongkorn University:

Professors,
Distinguished Participants,
Ladies and Gentlemen;

It gives me great pleasure to extend to you all a very warm welcome on behalf of Chulalongkorn University to Bangkok, Thailand, and to the Pure and Applied Chemistry International Conference 2016 (PACCON2016) during February 9 – 11, 2016. The PACCON2016 is held in conjunction with the Department of Chemistry, Faculty of Science, Chulalongkorn University, to celebrate the 100th year anniversary of the establishment of Chulalongkorn University.

Chemistry was one of the first disciplines offered at the Faculty of Science, Chulalongkorn University since the establishment of the university a century ago. It is, therefore, our great honour to showcase how far chemistry has come in Thailand during the past 100 years under the conference theme "THAILAND: One Hundred Years of Advancement in Chemistry".

The PACCON2016 will also provide a ground for learning about cutting-edge scientific discovery and innovation, discussing potential chemistry insights with experts from all over the world, as well as starting or strengthening collaboration across chemistry disciplines and sectors. I truly hope that friendship and knowledge obtained here will be long-lasting and lead to scientific breakthroughs in the near future.

Last but not least, I would like to express my sincere thanks to all plenary speakers, invited speakers and participants for their contributions; and to our sponsors, reviewers, organising committee and staff for putting in immense time and effort to make the PACCON2016 a memorable event. Our success here will be measured by how far chemistry can go in Thailand in the next 100 years, and I hope that you feel the same. I wish you an enjoyable stay in this warm and gorgeous, yet stimulating, city of Bangkok.

Associate Professor Dr. Polkit Sangvanich
Dean, Faculty of Science
Chulalongkorn University



Welcome Message



Welcome Message



Welcome Message from the Chairman of PACCON2016:

The Pure and Applied Chemistry International Conference (PACCON) was organized for the first time in 2002 by the Department of Chemistry, Faculty of Science, Chulalongkorn University. As part of the celebration of 100 years anniversary of the establishment of Chulalongkorn University, the Department of Chemistry once again will proudly be hosting the Pure and Applied Chemistry International Conference 2016 (PACCON2016), in conjunction with the Chemical Society of Thailand (CST) under the Patronage of Professor Dr. Her Royal Highness Princess Chulabhorn.

PACCON2016 will take place in Bangkok, Thailand during February 9 – 11, 2016 under the theme "THAILAND: One Hundred Years of Advancement in Chemistry". In keeping with the theme, PACCON2016 will feature 12 scientific sessions, 7 special sessions and 4 special activities, showcasing various aspects of how far pure and applied chemistry in Thailand have come in the past 100 years. The conference will be a common ground for scientists from all over the world to present new ideas, exchange experiences, gain insights in forefront chemistry research and education, and share entrepreneurial initiatives. Also, we would like PACCON2016 to be a place to promote collaborative arrangements in chemistry among different sectors of chemical research and education including industries, academia, research institutes, and government laboratories. More importantly PACCON2016 would strengthen collaborative network and friendship beyond boundaries.

Since its inauguration in 2002, the Pure and Applied Chemistry International Conference has emerged as one of the series of successful cosponsored international scientific conferences in the Asia-Pacific region. The Department of Chemistry, Faculty of Science, Chulalongkorn University would like to warmly welcome scientists of all generations from various disciplines and backgrounds around the world to Bangkok, Thailand in February 2016. We hope this will be a great opportunity for every participant to enjoy the superb science, the warm friendship, as well as the hard-to-beat natures in the Land of Smiles!

Associate Professor Dr. Vudhichai Parasuk
Chairman, Department of Chemistry
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Power model for enzymatic hydrolysis of coconut coir with chemical pretreatment

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Abstract:

Coconut coir, that contains cellulose, hemicellulose, lignin, and some other extractive compounds, is classified as complex lignocellulosic material. Glucose from coconut coir can be used as fermentation substrate after enzymatic hydrolysis. Lignin content from the coconut coir will act as an inhibitor in this hydrolysis process. Therefore, a pretreatment process is needed to enhance the hydrolysis of cellulose. It has been found out that; pretreatment methods have significant impact on production efficiency of ethanol from biomass. Some of the most promising pretreatment methods require the application of chemicals such as alkali, acids, salts, oxidants, and solvents.¹ In this research, chemical pretreatment, i.e. dilute acid and alkaline pretreatment were done prior to enzymatic hydrolysis of coconut coir. Previous study observed that the the best pretreatment was at 1.5% sulfuric acid concentration and 100 °C for dilute acid pretreatment² and 11% NaOH and 100 °C for alkaline pretreatment.³ Here, pretreatment was done at 121 °C and 11% NaOH; and 105 °C at 1.5% sulfuric acid. The objective of this research is to compare the glucose as a product of hydrolysis for these two types of chemical pretreatment. The kinetic parameters due to simple power model were then obtained.

1. Introduction

Fuel-ethanol production from sugar-cane, beet and corn may be a problem in the near future due to the food competition in the use of these materials for bioenergy production.⁴ Therefore, conversion of abundant lignocellulosic biomass to ethanol as a bio- fuel presents an important opportunity to improve energy security, reduce greenhouse gas emission, reduce the trade deficit, and improve price stability.⁵

Recently, several ways of utilizing biomass and associated waste for energy production in different forms e.g., bio-ethanol, biogas, bio-diesel, pyrolytic bio-oil, etc. have been envisaged thoroughly by researchers around the world.^{6,7,8}

Coconut coir (Figure 1) is lignocellulosic biomass. It is a natural fibre extracted from the husk of coconut and used in products such as floor mats, doormats, brushes, mattresses, etc. Coir is the fibrous material found between the

hard, internal shell and the outer coat of a coconut. As lignocellulosic biomass, coconut coir can produce second generation bioethanol in three main steps: pretreatment, hydrolysis, and fermentation.

Pretreatment involves the use of physical processes (e.g., size reduction, steaming/boiling, ultrasonication, and popping), chemical methods (e.g., acids, bases, salts, and solvents), physicochemical processes (e.g., liquid hot water and ammonium fibre explosion or AFEX), biological methods (e.g., white-rot/brown-rot fungi and bacteria), and several combinations thereof to fractionate the lignocellulose into its components.¹

Chemical pretreatment for coconut coir had been studied previously.^{2,3} It was found that the best pretreatment was at 1.5% sulfuric acid concentration, 100 °C for dilute acid pretreatment² and 11% NaOH, 100 °C for alkaline pretreatment.³

Power model was used to represent kinetic of the coconut coir batch enzymatic

hydrolysis under alkaline pretreatment.⁹ A comparison of this power model and the first order dynamic model had also been presented.¹⁰

The objective of this research is to compare the glucose as a product of hydrolysis for these two types of chemical pretreatment. The kinetic parameters due to simple power model were then can be obtained.



Figure 1. Coconut coir.

2. Materials and Methods

2.1 General

The methodology outline is shown in Figure 2.

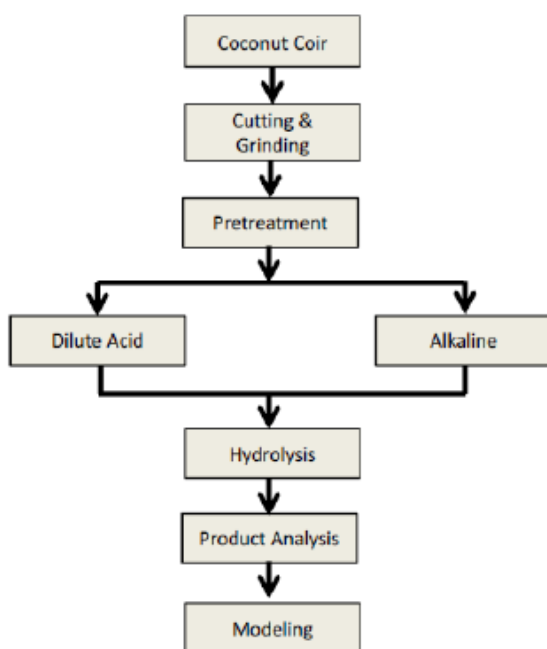


Figure 2. Methodology outline.

2.2 Cutting and Grinding

Coconut coir that had been cut into pieces milled using a disc mill. Then the material screened to 200 mesh.

2.3 Pretreatment

2.3.1 Dilute acid

Delignification carried out using sulfuric acid with a concentration of 1.5% w/w and a temperature of 105 °C for 60 minutes. The slurry concentration was 15% w/v and liquid volume of 350 mL.

2.3.2 Alkaline

This study used 11% NaOH and the temperature of 121 °C for 60 mins. The slurry concentration was 7.5% w/v. Then the solid filtered and washed to neutral pH.

2.4 Hydrolysis

The enzymatic hydrolysis were done for variation of 0.1; 0.2; 0.4; 1 and 2 grams of coconut coir and 0.6 mL of enzyme in a total volume of 100 mL. The hydrolysis using 250 mL erlenmeyer. The initial pH was made 4.8 with citrate buffer.

In order to avoid microorganism contamination, 40 µg/mL tetracycline antibiotic were added. Subsequently the mixture was incubated for 3 days at 50 °C in an incubator shaker with a rotary speed of 150 rpm. The experiment was performed three times for triplication. Enzymatic reaction was stopped by heating at 100 °C for 5 minutes. Then filtration is performed using a filter paper.

2.5 Product analysis

Reducing sugar analysis using DNS method.

2.6 Modeling

Data from the experiment were then modeled by the power model so that the model parameters can be determined. The following power model was used to match the curve of the product as a function of reaction time:⁹

$$P = a \times t^b$$

where: P = the resulting product (mg/L), t = reaction time (hour), a and b are empirical parameters.

3. Results & Discussion

Table 1 shows model parameters for various substrate concentration for both dilute acid and alkaline pretreatment. The models obtained were quite satisfactory in terms of the value R^2 approaching one. Figure 3 to 7 shows experimental and model results for variation of 0.1, 0.2, 0.4, 1 and 2 g/100 mL coconut coir respectively, for both dilute acid and alkaline pretreatment. As can be seen in those figures, dilute acid pretreatment gives higher reducing sugar than alkaline pretreatment.

Table 1. Parameters for power model.

Substrate Concentration [g/100 mL]	a	b	R^2
Dilute Acid:			
0.1	502.6	0.1715	0.9834
0.2	582.0	0.1355	0.9827
0.4	614.5	0.1284	0.9867
1.0	672.8	0.1216	0.9873
2.0	874.0	0.06046	0.9976
Alkaline:			
0.1	68.17	0.3137	0.9447
0.2	112.8	0.2549	0.9656
0.4	361.9	0.2206	0.9720
1.0	582.5	0.1180	0.9140
2.0	738.7	0.06981	0.8941

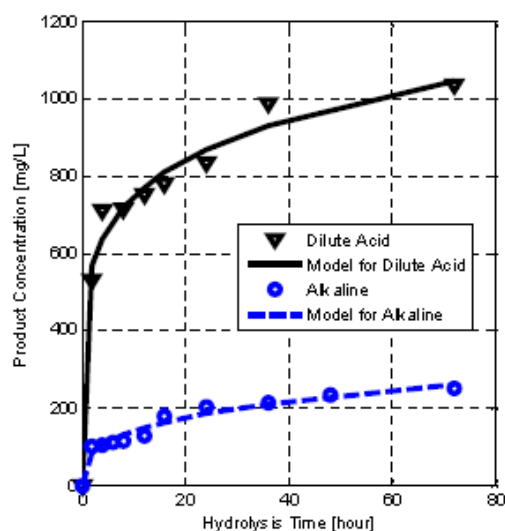


Figure 3. Results from 0.1 g/100 mL substrate.

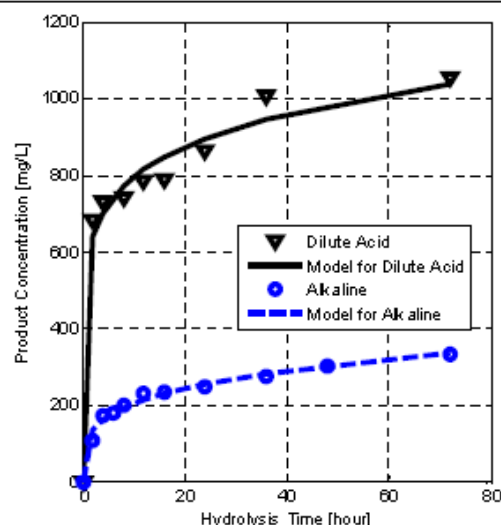


Figure 4. Results from 0.2 g/100 mL substrate.

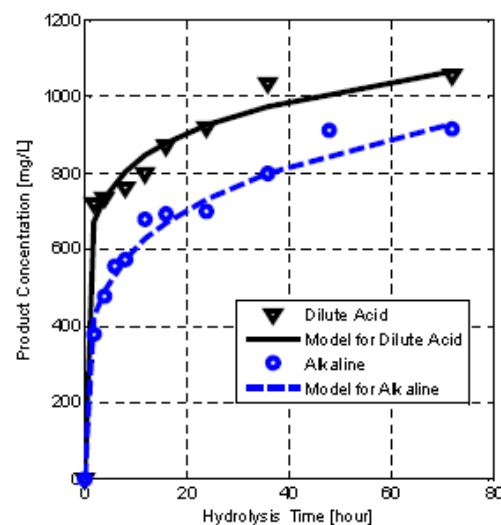


Figure 5. Results from 0.4 g/100 mL substrate.

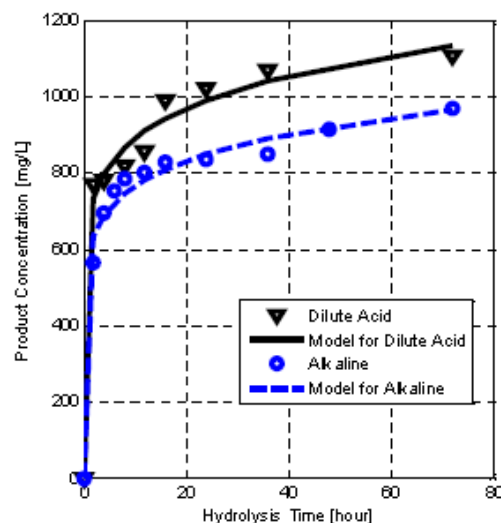


Figure 6. Results from 1.0 g/100 mL substrate.

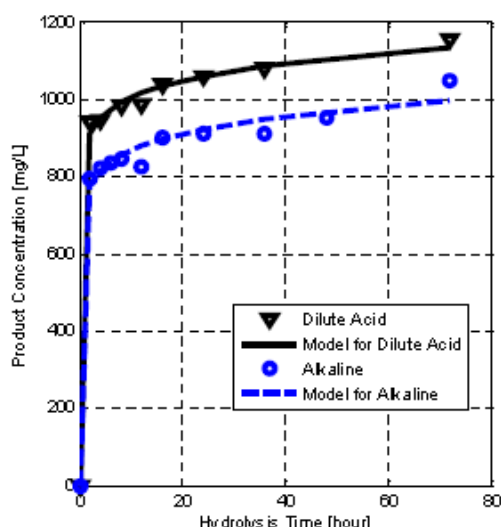


Figure 7. Results from 2.0 g/100 mL substrate.

4. Conclusion

Enzymatic hydrolysis of coconut coir with chemical pretreatment (i.e dilute acid and alkaline) has been done and produce reducing sugar. Simple empirical power model of batch hydrolysis reaction has been obtained (Table 1). It appears that dilute acid pretreatment is more promising than alkaline (Figures 3 to 7).

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