



UNIVERSITY OF
REGINA



Green Science and Technology Conference 2008 **Office of Energy and Environment (OEE)**

June 10, 2008

**Multipurpose Room, 150 - 10 Research Drive, Regina Research Park on
Campus**

Abstracts

<http://www.uregina.ca/greenconference2008/>

List of Abstracts

S.No	Title	Authors	Page No.
1.	A Personal Reflection on Environmentally Friendly Reaction Media	Richard M. Pagni	4
2.	Assessment and implementation of CO ₂ capture, transportation and storage for new large-scale fossil-fuel fired power plants	Richard Hotchkiss	5
3.	Chemicals from Biomass with Sub and Super Critical Fluids	S.N .Naik and A.K. Dalai	6
4.	Determination of kinetic parameters using distributed activation energy model for lignin pyrolysis	<u>Thilakavathi Mani</u> , Pulikesi Murugan, and Nader Mahinpey	7
5.	Ionic liquids, use and specific task as solvent in catalytic reaction	Santini Catherine C.	8
6.	LCA of Crude Oil associated with CO ₂ Post-Combustion Capture through CO ₂ EOR and Storage	J. Suebsiri, M. Wilson and P. Tontiwachwuthikul	9
7.	Novel Materials for Dispersive Solid Phase Extraction Applications	J. A. Kwon, S. T. Mahmud, M. O. Mohammed, and <u>L. D. Wilson*</u>	10
8.	Optimization of Kinetic parameters and 2-D Reactor Modeling for Simulation of the Catalytic Reduction of NO _x in the Monolith Honeycomb Reactor	S.R.Dhanushkodi, N.Mahinpey, and M.Wilson	11
9.	Pressurized Solvent Extraction of Neem (<i>Azadirachta indica</i> A. Juss) Seed Kernels for Azadirachtin rich extracts	G.C. Jadeja and S.N. Naik	12
10.	Preparation and Sorption Studies of Carbohydrate Polymers	<u>Dawn Y. Pratt</u> , Adel Sudom, Lee D. Wilson	13

11.	Structural characterization of char obtained from pressurized pyrolysis of wheat straw	<u>Pulikesi Murugan</u> , Thilakavathi Mani, and Nader Mahinpey	14
12.	Sorption Studies of Novel Polysaccharide-grafted Activated Carbon Materials	<u>Kwon, J. H.</u> and Wilson, L. D.	15
13.	Some Computational Chemistry Studies of Petroleum Cracking	<u>Allan L. L. East</u>	16
14.	Synthesis of Chemically Modified Vegetable Oils for Lubricant Applications	<u>Vaibhav V. Goud</u> and Ajay K. Dalai	17

A Personal Reflection on Environmentally Friendly Reaction Media

Richard M. Pagni*

Department of Chemistry, University of Tennessee, Knoxville, TN 37996

Abstract

There have been many important discoveries in the burgeoning field of green chemistry. Many well-established reactions can now be carried out in a variety of environmentally friendly ways, often in higher yields and shorter reaction times and at lower temperatures than their older counterparts. A pleasant discovery in green chemistry is that new reaction media often result in entirely new chemistry. This talk will consider examples from both categories, some taken from the literature and others from the author's own research.

Assessment and implementation of CO₂ capture, transportation and storage for new large-scale fossil-fuel fired power plants

Richard Hotchkiss
RWE npower R&D

Abstract

The United Kingdom faces twin challenges of carbon dioxide emissions and the need to replace old power plants which will soon have to close because of environmental legislation. This presentation will consider the position of one of the UK's electricity generation companies and its plans to meet the carbon dioxide challenges within an uncertain regulatory framework. The reasons for our approach will be discussed. Our submission for the UK Government carbon dioxide capture and storage competition will be discussed.

Chemicals from Biomass with Sub and Super Critical Fluids

S.N .Naik* and A.K. Dalai

Department of Chemical Engineering, University of Saskatchewan, Saskatoon Canada

*Email: san354@mail.usask.ca

Abstract

Global Environmental problems such as climate change, acid rain, water pollution, are due to excessive use of petroleum based fuels, chemicals, fertilizer, pesticides, detergent, lubricant, polymers. Therefore Chemical industries follows alternative pathways for design of chemical processes and products that will reduce or eliminate the use and generation of hazardous chemical substances to environment. In such situation, Biomass resources are becoming important alternative feedstock to replace fossil resources for production of chemicals and fuels. Plant biomass produced two types of organic chemicals, macro or primary metabolites (cellulose, hemicelluloses, starch, lignin) and micro or secondary metabolites (amino acids, alkaloids, terpenoids, etc.) which can be utilized for production of environmental friendly bio-products. Sub and super critical fluids (Carbon dioxide and Water) processing technology have been gaining attention as both an environmental benign attractive solvent and reaction medium for variety of applications. It is cheap, nontoxic, nonflammable, non explosive and offer advantages compared to other substances. This paper focus, the processing of biomass by using sub and super critical fluids for extraction of secondary metabolites and conversion of primary metabolites to fuels and chemicals.

Determination of kinetic parameters using distributed activation energy model for lignin pyrolysis

Thilakavathi Mani, Pulikesi Murugan, and Nader Mahinpey

Faculty of Engineering, University of Regina, SK, Canada, S4S 0A2

Abstract

Due to the scarcity of natural fuel resources and the abundance of biomass, the interest in the conversion of biomass into useful energetic products has been evolved. Lignin is one of the major components present in biomass that can be converted into bio-oil through thermochemical processes. To study the kinetics of complex reactions such as pyrolysis of biomass, the distributed activation energy model (DAEM) has been widely utilized. This model assumes a set of irreversible first-order reactions that have different activation energies. The function $f(E)$ was determined from the linear correlation obtained between $X(E)$ and E . As the conversion increases, activation energy also increases in the range from 6.5 to 27 kcal/mol. In this study, Simulated Annealing Method has been used for the determination of DAEM kinetic parameters for the non-isothermal pyrolysis of lignin using thermogravimetric analysis (TGA) data. Predicted results from the optimum kinetic parameters have been compared with the non-isothermal TGA data of lignin.

Ionic liquids, use and specific task as solvent in catalytic reaction

Dr SANTINI Catherine C.

Directeur de Recherche au CNRS
Université de Lyon, ICL, LC2P2
Equipe Chimie Organométallique de Surface
UMR 5265 CNRS-CPE lyon, France, santini@cpe.fr

Abstract

Our research field concerns the use of ionic liquids, as alternative media, in view of more sustainable chemical industry.¹

Ionic liquids are organic salts that are liquid at temperatures close to ambient. They are composed of voluminous organic ions characterized by molecular structures that are asymmetric and flexible with a delocalization of the electrostatic charges.² A large number of cation and anion combinations are possible, resulting in a large variety of ionic liquids with chosen properties adapted to their uses as solvents or reaction and catalysis media.³

In several catalytic reactions studied in our laboratory, such as the telomerisation of butadiene (Celanese), the isomerisation of 2-methyl-3-butenitrile into 3-pentenitrile (Rhodia), or the hydrocyanation of 3-pentenitrile in adiponitrile (Rhodia), we have shown that the ionic liquid could play other roles than that of an “innocent” solvent. It could behave as a catalyst itself, as a co-catalyst or as a catalyst activator, or even be the source of a new ligand for a catalytic metal centre.⁴

The aim is to contribute to the understanding of the specific role of the molecular and structural properties of ionic liquids on the nature of the catalyst and of the substrate and in their subsequent use in selective catalysis.

¹Parvulescu V. I. and Hardacre, C., *Chem. Rev.* **107**, 2615 (2007)

² Wasserscheid P. and Welton, T., (eds.), "*Ionic liquids in Synthesis*" Wiley-VCH, Weinheim, 2007

³ Welton, T., *Coordination Chem. Rev.* 2004, 248, 2459-2477

⁴(a) Vallee, C. *et al.*, *J. Mol. Catal.*, 2004, 214, 71-81; Vallee, C. *et al.*, *Adv. Synth. Catal.* 2005, 347, 1835-

1847; (b) Lecocq V. *et al.*, *New. J. Chem.*, 2005, 29, 700-706; (c) Lecocq V. *et al.*, *J. Mol. Catal.*, 2006, 246,

242-247; (d) Bibal C. *et al.*, *Dalton*, 2008 ; (e) Hintermair U; *et al.*, *J. organometal. Chem.*, 2008

LCA of Crude Oil associated with CO₂ Post-Combustion Capture through CO₂ EOR and Storage

Jitsopa Suebsiri¹, Malcolm Wilson¹ and Paitoon Tontiwachwuthikul

¹Office of energy and environment, University of Regina, Regina, Canada, S4S 7J7

²Faculty of Engineering, University of Regina, Regina, Canada, S4S 0A2

Abstract

The global trend towards the use of taxation and credit trading systems including international co-operation to encourage the use of various methods to reduce the emissions of CO₂ to the atmosphere will require the development and use of environmental management tools to better understand the implications for these reductions. Carbon capture and storage technology, one of the approaches for CO₂ emission reduction being given serious consideration globally, presents an opportunity to reduce greenhouse gas emissions from large point sources such as fossil fuel industries. CO₂ post-combustion capture technology, retrofitted to existing equipment, is basically one that removes CO₂ from the flue gas following the combustion of the fossil fuel. The advantages of this technique are not only the use of CO₂ to enhance oil recovery, but also the storage of CO₂ for the long term. Life cycle assessment (LCA), one of the well-known environmental management tools, is defined as a process inventory that can help regulators to formulate environmental legislation, assist manufacturers to analyze their processes and improve their products, and potentially enable consumers to make more knowledgeable decisions.

Therefore, the research objectives are to study and to analyze the implications of energy industry associated with CO₂ capture and storage for CO₂ emission reduction. Since fossil fuel industries are playing a significant role in energy balance for all over the world, especially crude oil and coal, this research focuses on applying life cycle assessment (LCA) of crude oil including a coal fire power plant with CO₂ post-combustion capture through the use of CO₂ for EOR and storage. Moreover, the research aims to identify opportunities to improve the reduction of CO₂ emission including the use of LCA associated with other environmental management tools, such as risk assessment and total cost accounting.

Novel Materials for Dispersive Solid Phase Extraction Applications

J. A. Kwon, S. T. Mahmud, M. O. Mohammed, and L. D. Wilson*

Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan,
S7N 5C9 Canada

Tel. 306-966-2961; Fax. 306-966-4730; Email: lee.wilson@usask.ca

Abstract

In this work, we report the synthesis, characterization, and the sorption properties of a series of supramolecular-based porous materials according to three different materials design strategies as follows: *i*) “bottom-up” approach, *ii*) grafting approach, and *iii*) grafted mesoporous frameworks. “Bottom-up” materials were prepared through various addition reactions between oligosaccharides and diisocyanates and by substitution reactions between oligosaccharides and epichlorohydrin. Grafted materials were prepared using carbon templates whereas mesoporous silica templates involved attaching oligosaccharides using an appropriate linker molecule. Spectrophotometry, NMR spectroscopy, and thermodynamic techniques were utilized for the structural and physical characterization of the supramolecular frameworks. The surface and pore structure characteristics of the materials were studied using nitrogen porosimetry. The sorption properties of these materials were estimated using a dye-based sorption method. The composite materials described in this research will contribute positively to applications that employ dispersive solid phase extraction of organic contaminants from aqueous solution.

Optimization of Kinetic parameters and 2-D Reactor Modeling for Simulation of the Catalytic Reduction of NO_x in the Monolith Honeycomb Reactor

S.R.Dhanushkodi¹, N.Mahinpey^{1,2}, M.Wilson³

¹Process Systems Engineering, University of Regina, Regina, Canada, S4S 0A2

²Environmental Systems Engineering, University of Regina, Regina, Canada, S4S 0A2

³Office of energy and environment, University of Regina, Regina, Canada, S4S 7J7

Abstract

Emission of NO_x is of primary environmental concern in the oil sands industry. Selective catalytic reduction (SCR) is one of the best NO_x reduction technologies. The present study discusses the developing and testing of a mechanistic kinetic model for the SCR of NO_x to describe the kinetics of V₂O₅/TiO₂ catalysis at atmospheric pressure and a temperature of 250,300,350 and 400°C in a monolith honeycomb reactor. The kinetic modeling results impart insight into the significance of the diffusion with reaction steps and guidance for optimal monolith design for SCR. Reaction kinetics for of SCR, highly-interconnected rate kinetic schemes is modeled using analytical solutions to a system of ordinary differential equations. The algorithm employs standard linear algebra methods that are implemented using Matlab and verified with solver tool in excel. In order to determine rate constants from experimental data, fitting algorithms using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) methods were implemented that adjust rate constants to fit the model to experimental data. A heterogeneous numerical model consisting of coupled mass and momentum balance equations was solved using the finite elements method without neglecting the axial dispersion term. The validated expression would predict the conversion performance of the catalysts for different values of temperature inlet and ammonia concentration. A good agreement between experimental and model results has been obtained. The operating range for the catalyst relies on the NO conversion and emission.

Pressurized Solvent Extraction of Neem (*Azadirachta indica* A. Juss) Seed Kernels for Azadirachtin rich extracts

G.C. Jadeja and S.N. Naik

Centre for Rural Development & Technology, Indian Institute of Technology Delhi.

Hauz Khas, New Delhi 110016 India

*snn@rdat.iitd.ac.in

Abstract

The evergreen Neem (*Azadirachta indica* A. Juss) tree, belonging to the Meliaceae family, is a storehouse of botanical pesticides owing to the presence of bioactive limonoids in seed kernels that possess antifeedant, growth disrupting and larvicidal properties against an array of agricultural pests. Pressurized Liquid Extraction (PLE), is fast emerging as an efficient means for recovering valuable active ingredients from natural plant matrices at an accelerated rate and with a reduced solvent consumption. The technique employing heated ecofriendly organic solvents at elevated pressures of up to about 200 bar is a potential substitute for conventional solvent extractions. The present study deals with the application of PLE to obtain azadirachtin rich extracts from defatted neem seed kernels (NSK). The influence of several important parameters like temperature, pressure, extraction time and particle size on the extract yield and azadirachtin content of the extract was studied. A comparative study with classical solvent extraction methods was conducted to highlight the superiority of PLE in terms of time of extraction, solvent usage and also extraction yield. The azadirachtin content in the extracts was determined by HPLC.

Preparation and Sorption Studies of Carbohydrate Polymers

Dawn Y. Pratt, Adel Sudom, Lee D. Wilson*

Department of Chemistry, University of Saskatchewan,
Saskatoon, Saskatchewan, S7N 5C9 Canada

Tel: (306)966-2961 **Email:** lee.wilson@usask.ca

Abstract

Supramolecular polymeric networks comprised of 1:15, 1:25 and 1:35 feed ratios of β -cyclodextrin (β -CD) cross-linked with epichlorohydrin (EP) were synthesized and characterised by N_2 porosimetry, FT-IR, ^{13}C NMR, UV-Vis and elemental analysis. The sorption properties in aqueous solution were studied using a UV-Vis dye molecule, para-nitrophenol (PNP), a model compound of typical organic pollutants found in industrial wastewater. Sorption experiments were studied with different isotherm models, at pH 4.6 at various temperatures of 22°C, 32°C and 42°C, and pH 10.3 at 22°C. The parameters of the solution isotherms, as well as the surface areas of the polymeric materials were determined. The sorption and thermodynamic properties are influenced by temperature and pH; these conditions reveal the best adsorption conditions for the polymeric materials with the target adsorbate. The results of this study will contribute to an efficient remediation strategy of industrial effluents using carbohydrate-based polymeric materials.

Structural characterization of char obtained from pressurized pyrolysis of wheat straw

Pulikesi Murugan, Thilakavathi Mani, and Nader Mahinpey

Faculty of Engineering, University of Regina, SK, Canada, S4S 0A2

Abstract

Scanning electron microscopy (SEM) is a potential technique for studying morphology of particles of solid fuels. The aim of this work is to study the morphology of char particles obtained after the pressurized pyrolysis of wheat straw. Pyrolysis of wheat straw was performed in a tubular reactor at constant temperature (500°C) with different pressures ranges from 10 psi to 40 psi. SEM images of wheat straw char visually suggest that the parent material is made of solid cells strongly bounded but with evident slits, which seems to continue inside the particle. The shape of the fiber is maintained with slightly deeper openings after devolatilization in the reactor. The increase in pyrolysis pressure leads to the formation of waves and pores on the surface. On an average, about 50% of the biomass is released as volatile compounds during pyrolysis in a very short time. This results in the softening of the solid matrix caused by the rapid heating up. At high pressures, the loss of cell structure can be ascribed to the melting of the cell structure. It is noted that the tar formation is high at 40 psi compared to other low pressures. Therefore, the formation of tar may be responsible for the melting of cell structure.

Sorption Studies of Novel Polysaccharide-grafted Activated Carbon Materials

[Kwon, J. H.](#) and Wilson, L. D. *

Department of Chemistry, University of Saskatchewan, Saskatoon,
Saskatchewan, Canada, S7N 5C9.

Tel. 306-966-2961, Fax. 306-966-4730, email: lee.wilson@usask.ca

Abstract

Activated Carbon (AC) was modified using conventional grafting techniques to produce a surface with appended cyclodextrin (CD) groups and a polysaccharide-grafted AC (PSAC) material, respectively. The covalent surface modification was concluded using Raman spectroscopy, TGA, and mass spectrometry. The pore structure characteristics were concluded from nitrogen porosimetry from a comparison of as received materials with covalently modified GAC. Methyl chloride uptake with AC and PSAC materials was evaluated using a thermodynamic method. These results provide a further understanding of the uptake of GHG onto surface modified AC materials.

Some Computational Chemistry Studies of Petroleum Cracking

Allan L. L. East

Department of Chemistry and Biochemistry, University of Regina, Regina,
Saskatchewan., Canada S4S 0A2

Abstract

Our group has been using computational chemistry to study chemical reaction mechanisms for hydrocarbon cracking. Johnson et al. have shown that ionic liquids can crack and oligomerize hydrocarbons at moderate temperatures, and one of our goals has been to see if this catalytic benefit results in simply lower reaction barriers, or a change in mechanism also. I will present recent results from our studies. A better understanding of the mechanism involved may lead to the ability to design an ionic-liquid-based catalyst that can provide a narrower product distribution.

Synthesis of Chemically Modified Vegetable Oils for Lubricant Applications

Vaibhav V. Goud and Ajay K. Dalai

Catalysis and Chemical Reaction Engineering Laboratories,
Department of Chemical Engineering, University of Saskatchewan,
Saskatoon,
SK, S7N 5A9, Canada

Phone +1-306-966-6511; Fax: +1-306-966-4777; Email: yvg333@mail.usask.ca

Abstract

Owing to the unfavorable impact on the environment of mineral oil-based lubricants, there has been a steady increase in the demand for biodegradable, environment-friendly lubricants. From an environment point of view, the use of renewable feedstock is of great interest. Although the vegetable oils have some advantages, they also have poor oxidation and low temperature stability. One of the ways to address this issue is the chemical modification of the unsaturation content in the oil. We report here the synthesis of series of structural modifications of vegetable oil. This can be done by the addition of different carboxylic acids and alcohols of various complexities to the double bonds. The ring opening reaction of epoxidised canola oil with different alcohols such as methanol, isobutanol, 1-decanol was carried out in presence of sulphuric acid as a catalyst. The reaction was monitored and products were confirmed by NMR, FTIR analysis to demonstrate the potential of these newly developed fluids for use as lubricants.