

# SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

Volume 25

Number 25 – 2017

ISSN 0104-5431

# International Cataloging Data on Publication (CIP)

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY: órgão de divulgação científica e informativa [recurso eletrônico] / SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY – Vol. 25, n. 25 (Dec. 2017)- . – Porto Alegre: Grupo Tchê Química, 2017 - Anual. Sistema requerido: Adobe Acrobat Reader. Modo de acesso: World Wide Web: <http://www.sbjchem.com> Descrição baseada em: Vol. 25, n. 25 (Dec. 2017). ISSN 0104-5431

1. Química. I. SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY.

CDD 500

# SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

Volume 25

Number 25 – 2017

ISSN 0104-5431

## Editor-in-chief

• Dr. Luis Alcides Brandini De Boni, Brazil, CORSAN, <u>deboni@tchequimica.com</u>

## **Technical editors**

- Dr. Eduardo Goldani, goldani@tchequimica.com
- Ketevan Kupatadze, Dr., <u>kupatadze@tchequimica.com</u>, Geórgia, ISU

## **Editorial Board**

- Rafael Rodrigues de Oliveira, Dr., oliveira@tchequimica.com, Brazil, Neoprospecta
- Teresa M. Roseiro Maria Estronca, Dr., <u>roseiro@tchequimica.com</u>, Portugal, UC.
- Marcos Antônio Klunk, Dr., <u>marcosak@edu.unisinos.br</u>, Brazil, UNISINOS.
- Dr. Francisco José Santos Lima, lima@tchequimica.com, Brazil, UFRN.
- Monica Regina da Costa Marques, Dr., <u>aguiar@tchequimica.com</u>, Brazil, UERJ.
- Rodrigo Brambilla, Dr., <u>brambilla@tchequimica.com</u>, Brazil, UFRGS.
- Gabriel Rubensam, Me., <u>grubensam@tchequimica.com</u>, Brazil, PUCRS.
- Andrian Saputra, PhD., <u>saputra@tchequimica.com</u>, University of Lampung, Indonesia

# SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

ISSN - 0104-5431 (Print)

Available at http://www.sbjchem.com

### Mission

The SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY is a double-blind peer review, open access, multidisciplinary journal dedicated to publishing high-quality content and is intended to fill a gap in terms of scientific information for Southern Brazil. We have set high standards for the articles to be published by ensuring strong but fair refereeing by at least two reviewers. The Journal publishes original research articles in all the fields of Engineering, Mathematics, Physics, Chemistry, Biology, Agriculture, Natural resource management, Pharmacy, Medicine, and others.

Occasionally the journal will include review papers, interviews, and other types of communications. It will be published mainly in English, and at present, there are no page charges.

We hope that this journal will provide a forum for the dissemination of high-quality research in Science and are open to any questions and suggestions.

The responsibility for the articles is exclusive to the authors.

### Correspondências

Rua Anita Garibaldi, 359/603. Bairro Mon't Serrat. CEP: 90450-001 Porto Alegre – RS. Brasil. Skype: tchequimica www.sbjchem.com southbchem@gmail.com

### INFLUENCE OF FAST PYROLYSIS WITH TEMPERATURE ON GAS, CHAR AND BIO-OIL PRODUCTION

### KLUNK, Marcos Antônio<sup>1\*</sup>; DASGUPTA, Sudipta<sup>2</sup>; DAS, Mohuli<sup>2</sup>

<sup>1</sup> University of Vale do Rio dos Sinos, Graduation Program in Mechanical Engineering <sup>2</sup> Department of Earth Sciences, IIT Bombay, India Federation

### ABSTRACT

Rice husk is among the products that stand out in use, and it is used as an alternative source of energy. The use of rice husk as biomass in the feeding of pyrolytic reactors for power generation and chemical products can reduce the environmental problem destination of this waste. The advantages of this process are in the proper disposal of this waste and energy generation. Fast pyrolysis of the rice husk was carried out in temperatures of 400-600°C. This work aims to evaluate the influence of temperature on yield and product composition of the gas, bio-oil, and char. The yield of bio-oil proved to be efficient (62 wt.% at 450°C) due to the high heat transfer and mass, as well as the residence time in the reactor. In addition, bio-oil production decreases slightly due to increased gas yield (1 to 15 wt.%) as the temperature increases in the range of 400-600°C, with the composition being severely affected, i.e., The concentration of CO increases and that of CO<sub>2</sub> decreases. In addition, a slight increase in the concentration of CH<sub>4</sub> and C<sub>2</sub>-C<sub>4</sub> hydrocarbons occurs with increasing temperature. The yield of char at 400°C and 600°C was 41.14-34.77 wt.%, respectively, corresponding to a decrease of 16 wt.%. The char obtained is of low heating value but has good features for the production of active carbons and amorphous silica. These results demonstrate the efficiency and optimization of the fast pyrolysis of rice husk, in order to obtain biooil and char.

#### Page - 1

# THE USE OF X-RAY MICROTOMOGRAPHY TO ASSESS CHANGES IN THE VOIDS STRUCTURE OF ROCKS

# PONOMAREV, Andrei Aleksandrovich<sup>1</sup>; BUBNOVA, Aleksandra Vladimirovna<sup>2</sup>; KLUNK, Marcos Antônio<sup>3</sup>;

<sup>1.2</sup> Tyumen Industrial University, Department of Geology of Oil and Gas Fields <sup>3</sup> University of Vale do Rio dos Sinos, Graduation Program in Mechanical Engineering.

### ABSTRACT

The oil and gas industry is developing rapidly. Based on this, it is necessary to determine new methods of productive prospecting of mineral deposits. One of the most high-tech and perspective methods is computer X-ray microtomography. For this stage, this method is widely used for the different fields of geology and geophysics. The main advantage is the ability to study the sample without destruction, which is especially important in the process of working with the kern material. In this paper, the method of computerized X-ray microtomography is highlighted. A comparative analysis of the voids structure of an oil source rock before and after exposure to microwave fields using the standard DataViewer software is clarified. As a result of this analysis, an increase in the diameter of a sample of a cylindrical shape after treatment with microwave fields was established, and the formation of microcracks was also established. Based on the results obtained, assumptions were made about the formation of hydrocarbon deposits. In other words, the paper discusses in detail the method that allows fixing changes in the structure of the void space of rocks as a result of oil and gas generation flowing under the influence of wave fields.

#### Page - 12

# TIME, ENERGY EFFICIENCY IN THE PRODUCTION OF BIODIESEL, AND PRODUCTS DESTINATION IN A BIOREFINERY

#### DE BONI, Luis Alcides Brandini<sup>1</sup>;

<sup>1</sup> Southern Brazilian Journal of Chemistry

### ABSTRACT

This manuscript deals with the production of biodiesel from triglycerides (TG); soybean oil was the primary raw material. The transesterification reaction was used to convert triglycerides into monoalkyl esters. The catalytic mixture of methanol and potassium hydroxide (KOH) was used in the transesterification reaction. The anhydrous refining of biodiesel was used to reduce side reactions during the purification process. The treatment of glycerol by acidification with H3PO4 and its subsequent purification was a convenience process aiming to form the desired byproducts. The

conversion of residual fatty acids to soaps through the saponification reaction or into esters through the esterification reaction with H2SO4 can be done observing the market of those products. The monitoring of the transesterification reaction in real time with laser spectroscopy allows the variation of the temperature during the reaction process without losing the reaction endpoint. The use of only one reaction vessel for the accomplishment of several unit operations aiming the reducing of the reaction time in the production process was well succeeded. The main resulting products are biodiesel, glycerol, fertilizer, and soaps. As expected the biodiesel can be used as a source of energy, the glycerol can be further refined but this process was not explored at this manuscript, the resulting salts can be used as fertilizers, and the soups can be sold and used as a soup.

### Page - 17

# ARSENIC SPECIATION IN GROUNDWATER USING THE SOFTWARES PHREEQC, GWB AND GEODELING

# KLUNK, Marcos Antônio<sup>1\*</sup>; PONOMAREV, Andrey Alexandrovich<sup>2</sup>; DASGUPTA, Sudipta<sup>3</sup>; DAS, Mohuli<sup>3</sup>;

<sup>1</sup> University of Vale do Rio dos Sinos, Graduation Program in Mechanical Engineering <sup>2</sup> Tyumen Industrial University, Department of Geology of Oil and Gas Fields, Tyumen – Russian Federation <sup>3</sup> Department of Earth Sciences, IIT Bombay, India Federation

## ABSTRACT

Geochemical modelling speciation is used to understand the interactions that occur in the groundwater. Thermodynamic data, kinetic parameters, numerical methods are factors that affect any geochemical modelling system. The conceptual formulation of geochemical modeling calculates the distribution of chemically reactive species for an aqueous solution. The mathematical formulation of the model results in a system of nonlinear algebraic equations that are solved using numerical methods. Most programs allow the user to estimate the speciation model. Activities of aqueous species are usually calculated using the Davies equation, Debye-Hückel equation, or the extended Debye-Hückel equation. We perform a comparative study of geochemical speciation using three different software: PHREEQC<sup>™</sup>, Geochemist's Workbench<sup>™</sup> (GWB) and GEODELING. Details of each software take into account the distribution, mobility, and availability of chemical species in groundwater. We can observe very similar results in speciation when working with low-temperature systems (20 to 80°C). GWB™, PHREEQC™, and GEODELING employ an integrated system to define when to use Davies, Debye-Huckel or Bdot equation, according to the value of the solution ionic strength. The geochemical speciation aimed to compare the results of simulators able to predict the chemical species present in groundwater. The utilization of GEODELING allows comparing the results with software GWB™ and PHREEQC<sup>™</sup> with a high degree of acceptance for low temperatures. The numerical methods used by GWB<sup>™</sup>, PHREEQC<sup>™</sup>, and GEODELING software are able to seek its own best set of numerical solutions to achieve the equilibrium. Users must be cautious when choosing geochemical modeling software, as an essential factor for choosing a simulator is to know the temperature range that will be used.

### Page - 30

#### **TO AUTHORS**

Preparation of Manuscripts	 36
Guidelines for publication	 39
How to submit a manuscript?	 39