Romanian Chemical Engineering Society
Romanian Chemical Society
Academy of Technical Sciences – Chemical Engineering Section
University POLITEHNICA of Bucharest

SICHEM 2016
Book of Abstracts
Supplement

University Politehnica of Bucharest, Romania
September 8 – 9, 2016

Scientific Committee

Șerban AGACHI, *"Babeș-Bolyai" University Cluj-Napoca*, *ASTR*
Petru ILEA, *"Babeș-Bolyai" University Cluj-Napoca*
Alexandru OZUNU, *"Babeș-Bolyai" University Cluj-Napoca*
Liviu LITERAT, *"Babeș-Bolyai" University Cluj-Napoca*, *ASTR*
Cristian Călin CORMOȘ, *"Babeș-Bolyai" University Cluj-Napoca*
Mircea Vasile CRISTEA, *"Babeș-Bolyai" University Cluj-Napoca*
Liana Graziella TURDEANU, *"Babeș-Bolyai" University Cluj-Napoca*

Maria GAVRILESCU, *"Gheorghe Asachi" Technical University of Iași*
Dan CAȘCAVAL, *"Gheorghe Asachi" Technical University of Iași*
Ilie SIMINICEANU, *"Gheorghe Asachi" Technical University of Iași*, *ASTR*
Ioan MĂMĂLIGĂ, *"Gheorghe Asachi" Technical University of Iași*
Ionel Marcel POPA, *"Gheorghe Asachi" Technical University of Iași*
Silvia CURTEANU, *"Gheorghe Asachi" Technical University of Iași*

Corneliu DAVIDESCU, *Politehnic University of Timișoara*, *ASTR*
Delia PERJU, *Politehnic University of Timișoara*, *ASTR*
Teodor TODINCĂ, *Politehnic University of Timișoara*
Lucian Mircea RUSNAC, *Politehnic University of Timișoara*

Caludia KONCSAG, *Ovidius University of Constanța*
Irina NIȚĂ, *Ovidius University of Constanța*
Timur CHIS, *Ovidius University of Constanța*

Ion ONUȚU, *Petroleum – Gas University of Ploiești*

Denisa NISTOR, *"Vasile Alecsandri" University of Bacău*
Lucian GAVRILĂ, *"Vasile Alecsandri" University of Bacău*

Philippe MICHAUD, *Blaise Pascal University, Clermont-Ferrand*
Cédric DELATTRE, *Blaise Pascal University, Clermont-Ferrand*

Gholamreza DJELVEH, *SIGMA Clermont-Ferrand*
Fabrice GROS, *SIGMA Clermont-Ferrand*

Mihail BARBOIU, *European Institute of Membranes, Montpellier*
Jose Marcano SANCHEZ, *European Institute of Membranes, Montpellier*

Inmaculada Rodriguez RAMOS, *Institute of Catalysis and Petrochemistry*, *Madrid*

Ecaterina ANDRONESCU, *University POLITEHNICA of Bucharest*, *ASTR*
Sorin ROȘCA, *University POLITEHNICA of Bucharest*, *SChR*, *ASTR*
Horia IOVU, *University POLITEHNICA of Bucharest*
Ioan CĂLINESCU, *University POLITEHNICA of Bucharest*
Gheorghița JINESCU, *University POLITEHNICA of Bucharest*, *ASTR*
Grigore BOZGA, *University POLITEHNICA of Bucharest*, *ASTR*
Valentin PLEȘU, *University POLITEHNICA of Bucharest*
Vasile LAVRIC, *University POLITEHNICA of Bucharest*
Anicuța STOICA, *University POLITEHNICA of Bucharest*
Marta STROESCU, *University POLITEHNICA of Bucharest*
Dănuț-Ionel VĂIREANU, *University POLITEHNICA of Bucharest*
Tănase DOBRE, *University POLITEHNICA of Bucharest*, *ASTR*

NANOSTRUCTURED MATERIALS BASED ON COLLAGEN AND HYDROXYAPATITE USED TO BONE REGENERATION

Alexandra Elena OPREA[1*], Anton FICAI[1], Bogdan Ştefan VASILE[1],
Alexandru Mihai GRUMEZESCU[1], Ecaterina ANDRONESCU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials
Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Millions of patients suffering from various bone defects, most often derived from tumors or trauma. In last years, a lot of researchers have done thorough investigations on materials that present high potential to regenerate bone tissue by initiating a natural process of regeneration. Bone tissue is a natural nanocomposite material; an organic matrix consisting of collagen and inorganic salts (hydroxyapatite crystals), which provides mechanical support and protect vital organs and reserves of calcium and phosphate for the human body [1]. The intrinsic ability of bone regeneration without scarring is also known. An ideal material for bone reconstruction should be biocompatible, bioactive, to be able to initiate osteogenesis, and have similar properties to natural bone [2]. The aim of this work was to obtain, to characterize from physico-chemical and biological point of view different nanostructurated bioactive materials based on collagen and hydroxyapatite with potential application in hard tissue reconstruction and regeneration. A detailed approach about the synthesis and characterization is presented. Nanostructurated hydroxyapatite was obtained by precipitation and the dispersed in a collagen gel. The following methods were used for characterization: XRD, IR, SEM, TEM, SAED. The in vitro evaluation of biocompatibility was performed by monitoring two cell lines: stem cells and dermal fibroblasts. Also, two type of tests were performed for in vivo experiments: biodistribution evaluation of prepared composite and evaluation of bone regeneration potential. All tests demonstrate the high potential of collagen-hydroxyapatite composite for their use as potential material for filling and reconstruction of bone defects.

Keywords: hydroxyapatite, collagen, bone tissue, TEM, SAED, SEM, in vitro, in vivo.

References
[1] Kikuchi M., Hydroxyapatite/collagen bone-like nanocomposite, *Biol. Pharm. Bull.*, 36(11), 1666-9, 2013.
[2] Amini A. R., Laurencin C. T., Nukavarapu S. P., Bone Tissue Engineering: Recent Advances and Challenges, *Critical reviews in biomedical engineering*, 40(5), 363-408, 2012.

---

* Corresponding author: elena_oprea_93@yahoo.co.uk

SILICA NANOPARTICLES AS EFFICIENT VEHICLE FOR THE NATURAL COMPOUNDS

Bianca BOARCA[1*], Alina Maria HOLBAN[1,2], Bogdan Ştefan VASILE[1], Alexandru Mihai GRUMEZESCU[1], Ecaterina ANDRONESCU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*
[2]*Department of Microbiology–Immunology, Faculty of Biology, University of Bucharest, 36-46 Mihail Kogalniceanu Blvd, 050107, Bucharest, Romania*

We report the fabrication of a drug delivery system composed of SiO_2 loaded with three different essential oils (eucalypt, orange, cinnamon). The obtained materials have been physico-chemically characterized by infrared spectroscopy, X-Ray diffraction, scanning electron microscopy, transmission electron microscopy, Brunauer–Emmett–Teller analysis and thermogravimetric analysis. In vitro biological assays have been performed in order to evaluate the influence of the biomaterial on three different microbial stains (Staphylococcus aureus, Escherichia coli, Candida albicans), and, also, their biocompatibility [1,2]. IR spectra revealed the presence of all chemical groups specific to both SiO_2 and essential oils. XRD patterns show a characteristic diffraction interference to SiO_2 with reduced crystallinity. SEM micrographs reveal spherical morphology of the silica, relatively uniform distribution of particles and a tendency to form aggregates. The recorded TEM images show a spherical morphology. BET analysis presents a type IV isotherm in the case of simple SiO_2 and prove that the functionalization of SiO_2 with essential oils was successfully done. TGA show the amount of each essential oil that interacts with the SiO_2 network. Also, the biocompatibility tests revealed a good compatibility. The obtained SiO_2 proved to be an efficient vehicle for the natural compounds, the system proving to have inhibitory activity on S. aureus, E. coli and C. albicans biofilm development. The results show a great potential for a developing a new medication, in order to replace traditional antibiotics in the prevention and treatment of severe bacterial and fungal infections.

Keywords: silica nanoparticles, eucalypt, orange, cinnamon, XRD, TEM, TGA, antimicrobial effect.

References
[1] Voicu G., Dogaru I., Meliţă D., Meştercă R., Spirescu V., Stan E., Tote E., Mogoantă L., Mogoşanu G. D., Grumezescu A. M., Truşcă R., Vasile E., Iordache F., Chifiriuc M. C., Holban A. M, Nanostructured mesoporous silica: new perspectives for fighting antimicrobial resistance, *Journal of Nanoparticle Research*, 17, 201, 2015.

---

* Corresponding author: biancaboarca@yahoo.com

[2] Voicu G., Anghel A. G., Badea M., Bordei E., Crantea G., Gavrila R. I., Grecu A., Jercan D. A. M., Nicolae B. C., Vochitoaia G. C., Tchinda K., Holban A. M., Bleotu C., Grumezescu A. M., Silica network improve the effect of fludarabine and paclitaxel on HCT8 cell line, *Romanian Journal of Morphology and Embryology*, 55(2 Suppl), 545, 2014.

ZINC OXIDE THIN COATING USED AS ANTI-BIOFILM SURFACE

Mihaela-Loredana PANDEL[1*], Alina Maria HOLBAN[1,2], Anton FICAI[1],
Bogdan Ştefan VASILE[1], Alexandru Mihai GRUMEZESCU[1],
Ecaterina ANDRONESCU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*
[2]*Department of Microbiology–Immunology, Faculty of Biology, University of Bucharest, 36-46 Mihail Kogalniceanu Blvd, 050107, Bucharest, Romania*

Given that a large diversity of bacteria are resistant to drug treatment [1], this paper propose to test anti-biofilm character of ZnO thin coatings deposited by MAPLE technique [2]. The ZnO nanoparticles and the thin films surface were analysed by different methods (TEM, SAED, SEM, IR, XRD). Also, in order to highlight the effect of ZnO against bacterial colonization, both *in vitro* and *in vivo* experiments were carried out. The results showed that thin coating based on ZnO nanoparticles is biocompatible and presents intrinsic properties of anti-adherence acting against biofilm formation.

Keywords: anti-biofilm, zinc oxide, nanoparticles, MAPLE, bacterial colonization

References
[1] Rădulescu M., Andronescu E., Cirja A., Holban A. M., Mogoantă L., Bălşeanu T. A., Cătălin B., Neagu T. P., Lascăr I., Florea D. A., Grumezescu A. M., Dyia H. M., Chifiriuc M. C., Bolocan A., Antimicrobial coatings based on zinc oxide and orange oil for improved bioactive wound dressings and other applications, *Romanian Journal of Morphology and Embryology*, 57, 107, 2016.
[2] Oprea A. E., Pandel L. M., Dumitrescu A. M., Andronescu E., Grumezescu V., Chifiriuc M. C., Mogoantă L., Bălşeanu T. A., Mogoşanu G. D., Socol G., Grumezescu A. M., Iordache F., Maniu H., Chirea M., Holban A. M., Bioactive ZnO coatings deposited by MAPLE – an appropriate strategy to achieve efficient anti-biofilm surfaces, *Molecules*, 21, E220, 2016.

---

[*] Corresponding author: loredana.pandel@yahoo.com

NANOSTRUCTURES BASED ON ZnO AND PHYTOCHEMICAL SUBSTANCES WITH COSMETIC APPLICATIONS

Vera Alexandra SPIRESCU[1*], Bogdan Ştefan VASILE[1], Alexandru Mihai GRUMEZESCU[1], Ecaterina ANDRONESCU[1]

[1]*Department of Science and Engineering of Oxide Materials and Nanomaterials, Faculty of Applied Chemistry and Materials Science, University POLITEHNICA of Bucharest, Polizu Street no 1-7, 011061, Bucharest, Romania*

The aim of this work was to prepare sunscreens based on ZnO, beeswax, shea butter, coconut oil and phytocomponents, noted Solange (for unfunctionalized ZnO) and Solange L (for functionalized ZnO). The method used to obtain the UV filter, nanostructured zinc oxide, was a sol-gel process, which allows obtaining a pure powder, without the necessity of further calcination, with optimal nanoparticle dimensions for the selected application [1,2]. A part of the obtained nanopowder was functionalized with limonene, a phytochemical substance, for the observance of changes in smell and UV absorption of the final product (the sun lotion). Regarding the crystalline structure, the resulted material showed a hexagonal wurtzite-type structure, typical for zinc oxide, with a preferential orientation (0 0 2) and free of detectable secondary phases through XRD. The zinc oxide was tested and analyzed by XRD, SEM, TEM, EDAX, IR, TGA, ZETA potential, the in vivo evaluation of distribution and the antimicrobial profile. It was noticed that the zinc oxide is optimal for the chosen application in the cosmetic industry. Solange and Solange L were made from simple ingredients (beeswax, shea butter, coconut oil and simple and (un)functionalized ZnO nanoparticles). After the execution, the creams were tested for UV absorbance which is the most important characteristic for sunscreen. It was observed that the creams have a very good UV absorbance, through the entire UV spectrum. The zinc oxide is an inorganic UV filter that constantly absorbs through the entire UV spectrum, to ~380 nm.

Keywords: sunscreens, zinc oxide, UV filter, TEM, beeswax, shea butter.

References
[1] Oprea Stoica A., Andronescu E., Ghitulica C. D., Voicu G., Grumezescu A. M., Popa M., Chifiriuc M. C., Preparation and characterization of undoped and cobalt doped ZnO for antimicrobial use, *International Journal of Pharmaceutics*, 510, 430, 2015.
[2] Stan M. S., Constanda S., Grumezescu V., Andronescu E., Ene A. M., Holban A. M., Vasile B. Ş., Mogoantă L., Bălşeanu T. A., Mogoşanu G. D., Socol G., Grumezescu A. M., Dinischiotu A., Lazar V., Chifiriuc M. C., Thin coatings based on ZnO@C18-usnic acid nanoparticles prepared by MAPLE inhibit the development of Salmonella enterica early biofilm growth, *Applied Surface Science*, 374, 318, 2015.

---

* Corresponding author: veraspirescu@gmail.com

SILICA NANOPARTICLES FOR ANTIMICROBIAL THERAPY

Eliza TOTE[1*], Alina Maria HOLBAN[1,2], Anton FICAI[1], Bogdan Ştefan VASILE[1], Alexandru Mihai GRUMEZESCU[1], Ecaterina ANDRONESCU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*
[2]*Department of Microbiology–Immunology, Faculty of Biology, University of Bucharest, 36-46 Mihail Kogalniceanu Blvd, 050107, Bucharest, Romania*

In this paper, we synthesized by templating silica nanostructures using TEOS (tetraethyl orthosilicate) as a precursor of silica and PVP (polyvinyl pyrrolidone) as a templating agent. The silica network was subjected to calcination in order to remove the PVP and obtaining ordered pores. Subsequently, the silica network was loaded with therapeutic agents (kanamycin and tetracycline) in order to evaluate the antimicrobial profile [1]. The antimicrobial activity was evaluated by Gram-positive and Gram-negative bacteria. SiO_2 microspheres resulting from the synthesis were characterized by scanning electron microscopy, EDAX, X-ray diffraction and IR microscopy. Also, tests were carried out in order to study the adhesion of cells to an inert substrate. Because of ordered porosity, high biocompatibility and antimicrobial effect demonstrated, this type of nanostructured silica can be used as an effective transporter and releaser of the therapeutic agent, reducing the amount of antibiotics necessary to eradicate an infection. Because of the anti-adherent properties throughout the tested concentrations of E. coli strain, the obtained hybrid material shows a remarkable potential for obtaining medical surfaces with anti-biofilm properties.

Keywords: silica, template, nanostructure, antimicrobial, PVP.

References
 [1] Balaure P. C., Popa R. A., Grumezescu A. M., Voicu G., Radulescu M., Mogoantă L., Bălşeanu T. A., Mogoşanu G. D., Chifiriuc M. C., Bleotu C., Holban A. M., Bolocan A., Biocompatible hybrid silica nanobiocomposites for the efficient delivery of anti-staphylococcal drugs, *International Journal of Pharmaceutics*, 510, 532, 2016.
[2] Voicu G., Dogaru I., Meliță D., Meştercă R., Spirescu V., Stan E., Tote E., Mogoantă L., Mogoşanu G. D., Grumezescu A. M., Truşcă R., Vasile E., Iordache F., Chifiriuc M. C., Holban A. M., Nanostructured mesoporous silica: new perspectives for fighting antimicrobial resistance, *Journal of Nanoparticle Research*, 17, 201, 2015.

---

[*] Corresponding author: tote.eliza@gmail.com

BIOACTIVE NANOSTRUCTURED MATERIALS BASED ON MAGNETITE AND PHYTOCOMPONENTS WITH APPLICATIONS IN ANTI-INFECTIOUS THERAPY

Iulia LUNGU[1*], Alina Maria HOLBAN[2], Bogdan Ştefan VASILE[1],
Alexandru Mihai GRUMEZESCU[1], Ecaterina ANDRONESCU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*
[2]*Department of Microbiology–Immunology, Faculty of Biology, University of Bucharest, 36-46 Mihail Kogalniceanu Blvd, 050107, Bucharest, Romania*

The development rate of microbial resistance for the current antibiotic is significantly bigger than the rate at which new antibiotics are produced [1]. Therefore, the need for development in this field is highly required. Magnetite nanoparticles received a lot of attention due to their wide applications in biomedicine. Their most important property is that they can be controlled by means of an external magnetic field directly to the desired site, therefore considerably diminishing the side effects on the surrounded areas [2]. In order to obtain a nanostructured system for anti-infectious therapy, the magnetite nanoparticles can exhibit antimicrobial properties by coating them with natural compounds obtained from plants.

The magnetite nanoparticles were easily synthesized by the co-precipitation method. The functionalization of these nanoparticles with phytocomponents (eugenol and carvone) was made in situ. The resulted nanoparticles have been characterized by infrared spectroscopy (IR), x-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and thermogravimetric analysis (TGA). The results showed that the nanoparticles had sizes between 5 and 12 nm with the tendency to form aggregates and were spherical shaped. XRD and IR confirmed the presence of the functionalized nanoparticles. The percentage of natural compound encapsulated on the surface of the nanoparticles was estimated through TGA, hence the quantity of eugenol being 2.688%, respectively carvone 1.766%. In order to analyze the antimicrobial effect of the nanosystem, in vitro testing were made on Gram-positive (Staphylococcus aureus) and Gram-negative (Pseudomonas aeruginosa) microorganisms. The results showed that the nanosystem inhibits significantly the biofilm development. Moreover, in vitro biocompatibility was tested and the results showed that none of the nanobiomaterials induced morphological changes in the diploid cells from the culture.

Key words: magnetite nanoparticles, eugenol, carvone, TGA, Gram-positive, Gram-negative, in vitro.

---

* Corresponding author: iulia.lunguu@gmail.com

References

[1] Grumezescu V., Andronescu E., Holban A. M., Mogoantă L., Mogoşanu G. D., Grumezescu A. M., Stănculescu A., Socol G., Iordache F., Maniu H., Chifiriuc C. M., MAPLE fabrication of thin films based on kanamycin functionalized magnetite nanoparticles with anti-pathogenic properties, *Applied Surface Science*, 336, 188, 2014.

[2] Liakos I., Grumezescu A. M., Holban A. M., Magnetite nanostructures as novel strategies for anti-infectious thepray, *Molecules*, 19, 12710-12726, 2014.

BIOCOMPATIBLE PROTECTIVE HAp–Ag COATINGS FOR TITANIUM IMPLANTS

Oana FUFĂ[1,2*], Gabriel SOCOL[2], Alexandru Mihai GRUMEZESCU[1],
Ecaterina ANDRONESCU[1], Roxana TRUȘCĂ[1], Bogdan Ștefan VASILE[1],
Marcela SOCOL[3], Roxana Cristina POPESCU[1,4], Alina Maria HOLBAN[1,5]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[2] *Lasers Department, National Institute for Laser, Plasma and Radiation Physics, Magurele, Atomistilor Street no 409, 077125, Magurele, Bucharest, Romania*

[3] *Laboratory of Optical Processes in Nanostructured Materials, National Institute of Materials Physics, Atomistilor Street no 405A, 077125, Magurele, Bucharest, Romania*

[4] *Life and Environmental Physics Department, "Horia Hulubei" National Institute for Physics and Nuclear Engineering, Reactorului Street no. 30, Magurele, Bucharest, Romania*

[5]*Microbiology and Immunology Department, Faculty of Biology, University of Bucharest, 36-46 Mihail Kogalniceanu Blvd, 050107, Bucharest, Romania*

Given the extensive use of titanium and its alloys for hard tissue restoration or replacement and the recent concerning data regarding their long-term-related unwanted effects, recent studies straightened their attention towards the experimental study of biocompatible protective coatings for titanium-based materials (with specific anti-wear, anti-corrosion, anti-inflammatory or anti-microbial activity), in order to fabricate novel titanium-based implantable devices with enhanced and long-term performance [1,2].

The aim of our experimental study was to produce bioactive and antimicrobial coatings consisting in commercial hydroxyapatite (HAp) and essential oil-functionalized silver nanoparticles (AgNPs) for titanium implants, by means of matrix assisted pulsed laser (MAPLE) technique. We firstly synthesized AgNPs functionalized with *Salvia officinalis* and *Cinnamomum aromaticum* essential oils by using a wet chemistry route, employing both classical and ultrasound-assisted synthesis. The as-obtained powdery samples were investigated in terms of composition and microstructure by TGA, FT-IR, XRD, SEM and TEM means. The *in vivo* biodistribution of the synthesized AgNPs was histologically evaluated by using a BALB/c mouse animal model. Subsequently, the obtained AgNPs were mixed with commercial HAp and deposited by MAPLE as composite coatings onto medical-graded titanium substrates. The compositional and microstructural features of the resulted films were investigated by means of IRM, XRD, SEM and AFM techniques. The biocompatibility of the HAp-AgNPs coatings was evaluated on osteoblast-like cells, by considering the cellular viability test, immunofluorescence assay and SEM analysis. The biofilm inhibitory potential of the obtained coatings against microbial pathogens was also assessed.

---

* Corresponding author: oana.fufa@inflpr.ro

Keywords: silver nanoparticles, hydroxyapatite, MAPLE, biocompatible, antimicrobial.

References
[1] Rădulescu M., Andronescu E., Holban A. M., Vasile B. S., Iordache F., Mogoantă L., Mogoşanu G. D., Grumezescu A. M., Georgescu M., Chifiriuc M. C., Antimicrobial nanostructured bioactive coating based on Fe_3O_4 and Patchouli oil for wound dressing, *Metals*, 6, 103, 2016.
[2] Rădulescu D., Grumezescu V., Andronescu E., Holban A. M., Grumezescu A. M., Socol G., Oprea A. E., Rădulescu M., Surdu A., Trusca R., Rădulescu R., Chifiriuc M. C., Stan M. S., Constanda S., Dinischiotu A., Biocompatible cephalosporin-hydroxyapatite-poly(lactic-co-glycolic acid)-coatings fabricated by MAPLE technique for the prevention of bone implant associated infections, *Applied Surface Science*, 374, 387, 2016.

MORPHOLOGICAL STUDIES ON CHEMICALLY MODIFIED ELECTRODES BASED ON (Z)-2-THIOXO-5-((4,6,8-TRIMETHYLAZULEN-1-YL)METHYLENE) THIAZOLIDIN-4-ONE

Maria Daniela POP[1*], Aida APAZ GHIULNARE[2], Dan BALAN[1], George BUICA[2], Eleonora-Mihaela UNGUREANU[1], Marius ENACHESCU[2]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*
[2] *Center for Surface Science and Nanotechnology, University POLITEHNICA of Bucharest Splaiul Independentei nr. 313, AN031, District 6, 060042*
Bucharest, ROMANIA

In this work, preparation and characterization of the polymer modified glassy carbon electrodes were reported. The Atomic Force Microscope (AFM) was used to investigate the morphological and mechanical properties of the deposited polymer layers onto glassy carbon electrodes. The imaged topographies of the analyzed samples exhibited the presence of some columnar shape features onto the layer surfaces. It was observed that, at constant charge, the surface roughness value of the deposited layers, which was calculated from the acquired topography images, increased with the increasing of the applied potential for EPC (P1, P2 and P3). At different charges, the roughness parameter showed the same behavior for the layers obtained applying a constant potential for EPC, without having a noticeable influence on the adhesive properties of these surfaces (samples P3, P4, P5 and P6 – about 24 – 26 nN). The two electrodes (P8 and P7) which were subjected to some extra treatments showed an increased value for the mean adhesion force compared to the others, about 38 nN, 32 nN, respectively. Furthermore, from the above mentioned samples, the electrode (P7) immersed in Pb aqueous solution has a lower mean adhesion force value (32 nN), probably due to the Pb contribution.

[*] Corresponding author: mariapop@msn.com

AUTHOR INDEX

Romanian Chemical Engineering Society
Romanian Chemical Society
Academy of Technical Sciences – Chemical Engineering Section
University POLITEHNICA of Bucharest

SICHEM 2016
Book of Abstracts

University Politehnica of Bucharest, Romania
September 8 – 9, 2016

Scientific Committee

THEORY OF SYSTEMS, PROCESS CONTROL, PAST, PRESENT AND FUTURE - THE WAY THEY GO ALONG WITH PROCESS ENGINEERING FOR SUSTAINABILITY

Paul Şerban AGACHI[1,2*]

[1] Department of Chemical, Material and Metallurgical Engineering, Botswana University of Science and Technology, Palapye, Botswana

[2] Chemical Engineering Doctoral School, University Babeş-Bolyai, Cluj-Napoca, Romania

The conference makes an excursion in the history of manufacturing and Process Control (PC) together with System Theory seen as interdependent. Starting with the development of the mankind, from its basic needs, going to the nowadays consumerist philosophy, the presentation describes the development of civilization from the Neolithic tool manufacturing to the present stage of intelligent manufacturing; it shows the necessity of improvement of approaching the processes from systemic point of view, then controlling them in order to improve the performances, efficiency, the environmental impact for a future sustainable development.

The history of *chemical products manufacturing* as the basis for the process engineering is described and in parallel, the steps forward of the *process control theories and practice* are presented.

Manufacturing processes are traced well back in the history of mankind long time before the antiquity. The Industrial Revolution (XVIIIth century) was the moment, the milestone, when the shift from batch to continuous processing occurred and incurred the development of the PC. The Industrial Revolution was the dawn of the consumerism stage in mankind's history and led to an unprecedented escalation in demand, both with regard to quantity and quality, for bulk chemicals such as sulfuric acid and soda ash. This meant two things: one, the size of the activity and the efficiency of operation had to be enlarged, and two, serious alternatives to batch processing, such as continuous operation, had to be examined. This created the need for an engineer who was not only understanding with how machines behaved, but also understood chemical reactions and transport phenomena [1,2]. Nowadays, *Process Engineering* is going on under the imperative of sustainable development with its consequences.

In parallel, the *Automatic Control* is a very fresh field of development. Of course, interest for small mechanical robots existed from the antiquity to the medieval times, the water clock being an example. But the Industrial Revolution was the inspiring period of the beginning of the process control (see Jacquard weaving looms, 18th century). Passing through Maxwell's analysis of the steam engine governor in 1868, the "primitive period of feedback control" finishes in 1900. It is standard to call the period from then until 1960 the *classical period of feedback control* and the period from 1960 through present times the *modern control* period. After 1970's, computers entered in the life of the process industries. The concept of examining the many parts of a complex

---

* Corresponding author: agachip@biust.ac.bw

process or plant together as a single unit, with all the interactions included, and devising ways to control the entire plant is called *Systems Engineering*. The conference introduces the beginnings of *System Theory* and the way it can facilitate the holistic understanding and approach of processes [3,4].

Keywords: Process Engineering, Process Control, Theory of Systems, Sustainability

References
[1] http://www.britannica.com/EBchecked/topic/108682/chemical-engineering/64679/History
[2] George E. Davies, https://en.wikipedia.org/wiki/George_E._Davis
[3] Agachi P. S., Cristea V. M., *Basic Process Engineering Control*, De Gruyter Gmbh, Berlin, Boston, Introduction, 2014.
[4] Mayr O., The origins of feedback control, *Scientific American*, Vol. 223, No.4 (October), 110-118, 1970.

PERVAPORATION OF AQUEOUS ETHANOL SOLUTIONS THROUGH PURE AND COMPOSITE CELLULOSE/BIOCELLULOSE MEMBRANES

Ali Al JANABI [1*], Al Sakini Ahmed HAMEED[1], Tanase DOBRE[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

The pervaporative (PV) performance in terms of total permeate flux, separation factor with respect to the separation of ethanol/water (EtOH/H_2O) was assessed for composite membrane based on cellulose dissolved in NaOH- thiourea solutions mixed with biocelluloes and tetraethyl orthosilicate (TEOS). The phase inversion method was employed for cellulose/biocellulose solution. The casting solution was spread as a thin film onto a glass plate (for nonsupported membranes) or a paper support (for supported membranes) and then exposed to ambient air for 24 h. NaOH-thiourea were removed from the film by treating with 1M HCl solution and rinsing with distilled water to a neutral pH, after that the rinsed membrane was kept in distilled water for 24 h and further dried at room temperature.
Two percent of biocellulose 10% and 30% with different operation temperature have been used in experiment. Pervaporation performances, which were evaluated in terms of total, permeate flux and pervaporation separation factor, strongly depended, biocellulose content, ethanol concentration and operation temperature. The experiment showed that the flux increases with decreasing the ethanol content and with increasing the operation temperature.

Keywords: alcohols dehydration, cellulose membrane, biocellulose membrane, permeate flux, pervaporation, separation factor

* Corresponding author: alialjanabi35@yahoo.com

NON-LINEARITY DISTRIBUTION OF NITROPHENOLS IN WATER-n-OCTANOL SYSTEM

Adriana RADU[1], Ali Al-JUBOORI[1], Ana Maria JOSCEANU[1], Daniel DINCULESCU[1*], Vasile LAVRIC[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Solid nitrophenols, were accurately weighed and contacted with different water: 1-octanol volume ratios for 24 hours, in stoppered glass flasks, placed in an orbital shaker. This contact time was considered long enough for reaching thermodynamic equilibrium. After phase separation, the amount of phenol in each phase was quantified by absorbance measurements. Variable path lengths were employed, as well as dilutions of certain organic samples to keep absorbance as high as 0.9. Calibration curves for nitrophenols in water saturated with 1-octanol were built, and their parameters were calculated by regression analysis.

The absorption spectra signaled the presence of both phenols and phenolates species, therefore a separate calibration curves for nitrophenolates in water saturated with 1-octanol were built. Again, the corresponding parameters were calculated by regression analysis.

The actual concentration of the nitrophenolates from spectral data collected in the 280 – 450 nm domain was accessible from the mass balance equation, as the absorption properties of nitrophenols in the given solvent were already known. The actual concentrations of nitrophenolates in the organic solutions varied between 4.3e-5 and 1.9e-4 M.

Keywords: nitrophenols partition coefficient, polar solvents, non-linear interractions

---

[*] Corresponding author: d_dinculescu@chim.upb.ro

CONCEPTUAL DESIGN OF PROPYLENE PRODUCTION BY METATHESIS OF 2-BUTENE

Andrei Maxim ANDREI[1], Costin Sorin BÎLDEA[1*]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

The demand for propylene is continuously increasing, due to its wide range of applications such as polypropylene, acrylonitrile, cumene, propylene oxide and other valuable products. Currently, the largest producers of propylene are fluid catalytic cracking (FCC) and naphtha steam cracking units. Although extensive research is being done for increasing the propylene yield in these latter units, alternative olefin conversion technologies should be considered for on-purpose propylene production. Examples are as propane dehydrogenation, olefin metathesis, methanol to propene and cracking low-value olefins.

In this contribution, the hierarchical methodology of process synthesis is applied to metathesis of 2-butene for propylene production. The metathesis of 2-butene is carried out in the presence of tungsten oxide catalyst, which converts butenes into valuable olefin products ranging from C2 to C6, particularly propylene. The by-product of fluid catalytic cracking unit (FCC), which contains mostly C4 olefins and is typically used in the LPG pool, is a low-cost feedstock for olefin metathesis. Several flowsheets are considered and analyzed. The results reveal the most effective alternative with respect to both economic and technical perspectives.

Keywords: propylene, 2-butene metathesis, process design

---

[*] Corresponding author: s_bildea@upb.ro

ASSESSMENT OF WATER QUALITY OF SMALL ARTIFICIAL LAKES IN THE BUCHAREST-ILFOV AREA

Ana-Maria ANGHEL[1*], Elena DIACU[2], György DEÁK[1], Cristina CIMPOERU[1], Ecaterina MARCU[1]

[1] *National Institute for Research and Development in Environmental Protection Bucharest, 294 Splaiul Independenţei, 6th District, 060031, Bucharest, Romania*
[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

The lakes are water bodies globally important and need to be assessed in accordance with the requirements of Water Framework Directive 60/2000/CE [1]. Small artificial lakes are discussed in this paper in terms of seven quality indicators: pH, total phosphorus (P_{tot}), biochemical oxygen demand (CBO_5), ammonia nitrogen ($N-NH_4^+$), nitrate nitrogen ($N-NO_3^-$), nitrite nitrogen ($N-NO_2^-$) and sulfate (SO_4^{2+}). Randomly were taken eleven samples from four small artificial lakes (numbered from L1 to L4) located in the Bucharest-Ilfov area during 2013-2015. The lakes are used especially for fishing, for this reason is necessary to monitor the mentioned indicators. From the computed basic statistic on 77 values [2] were obtained both perfect positive correlation and perfect negative correlation for the Pearson's correlation coefficient (*r*). Positive correlation was found between the following pairs of indicators: pH - CBO_5, $N-NH_4^+$ - $N-NO_2^-$, P_{tot} - SO_4^{2+}, CBO_5 - P_{tot}, pH - P_{tot}, SO_4^{2+} - CBO_5, pH - SO_4^{2+}, $N-NO_2^-$ - $N-NO_3^-$, SO_4^{2+} - $N-NO_3^-$, SO_4^{2+} - $N-NO_2^-$, P_{tot} - $N-NO_2^-$ and P_{tot} - $N-NO_3^-$. Strong positive correlation was found between the pair pH and CBO_5 with $r = 0.866$ and between P_{tot} - $N-NO_2^-$ a low positive correlation with $r = 0.023$. From the cluster analysis of variables of all indicators, six clusters were achieved. The high level of similarity was obtained between pH and CBO_5 with a percent of 93.33 and the lowest between $N-NO_3^-$ and ($N-NO_2^-$ - $N-NH_4^+$) with a percent of 45.86. For all analyzed water samples, the degree of contamination [3] was calculated and the value found was of 2.74. This value, together with all the other monitored indicators were used for the assessment of water quality, being thus possible to appreciate that in the monitored small artificial lakes the degree of contamination is low. The P_{tot} values ranged from 0.02 mg/L to 0.06 mg/L and indicate that the lake L1 is mesotrophic and the other three lakes are eutrophic according to Romanian Order no. 161 of 2006 [4]. According to the same legislative act, all the indicators fall within first class of water quality. The relationships established in this paper can contribute to a better understanding of the selected indicators in the evaluation of water quality of small artificial lakes.

Key words: artificial water bodies, nutrients, statistics, pollution indices

---

[*] Corresponding author: ana6209@yahoo.com

References

[1] Radu V. M., Diacu E., Ionescu P., Gy. Deák, Spatio-Temporal Characterization of Nutrient Pollution in Lower Danube Area, *Rev. Chem.*, 66(5), 601-606, 2015.

[2] Laboratories Department of National Institute for Research and Development in Environmental Protection Bucharest – INCDPM (*www.incdpm.ro*).

[3] Singh P. K., Verma P., Tiwari A. K., Sharma S., Purty P., Review of Various Contamination Index Approaches to Evaluate Groundwater Quality with Geographic Information System (GIS), *Int. J. ChemTech Res.*, 7(4),1920-1929, 2014-2015.

[4] Order no. 161 of 2006 – Norms on surface water quality classification in order to determine the ecological status of water bodies.

CONTRIBUTIONS REGARDING THE KINETICS OF LACTIC ACID FERMENTATION IN THE PRESENCE OF HYDROTALCITE

Vasilica Alisa ARU [1*], Oana Cristina PÂRVULESCU[2], Ileana Denisa NISTOR[1], Ana-Maria GEORGESCU[1], Gabriela MUNTIANU[1], Ana-Maria ROŞU[1], Nicoleta PLATON[1], Gheorghița JINESCU[2]

[1] *VASILE ALECSANDRI University of Bacău, Chemical and Food Engineering Department, 157 Mărăşeşti, 600115 Bacău, Romania*

[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

This paper presents a study of lactic fermentation kinetics in the presence of hydrotalcite. Experimental investigation was performed under static ($=0$) and ultrasonic ($=35$ kHz) operation conditions, at three values of operation temperature ($t_1=38°C$, $t_2=43°C$, $t_3=48°C$), and four values of solid (hydrotalcite)-liquid (milk) ratio ($R_0=0$, $R_1=1$ g_s/L, $R_2=5$ g_s/L, $R_3=7.5$ g_s/L). It was concluded that the final fermentation time, $_f$, was lower for static runs and decreased with t increasing and R decreasing. The best yoghurt quality, *i.e.* the most viscous and creamy coagulum with an insignificant syneresis and a maximum viable lactic bacteria concentration, was prepared at $=35$ kHz, $t=43°C$, and $R=5$ g_s/L. Due to a high content of viable LAB as well as to the presence of antacid clay, this yoghurt could have significant health benefits.

Key words: fermentation, lactic acid, ultrasound, yoghurt, hydrotalcite.

---

* Corresponding author: arusalisa@yahoo.com

THE IMPACT ASSESSMENT OF THE URANIUM INDUSTRY ON ENVIRONMENT

Diana BANU[1,2*], Viorica Elena IONI [2], Aura Daniela RADU[2], Mihai NI [3]

[1]*University of Bucharest, Faculty of Geology and Geophysics, 6 Traian Vuia Street, Bucharest, Romania*

[2] *Research & Development National Institute for Metals and Radioactive Resources, 70 Carol I Bvd., 020917, Bucharest, Romania*

[3] *University of Bucharest, Faculty of Physics, 405 Atomistilor Street, Magurele, Ilfov, Romania*

The activity of uranium mineralization exploration and exploitation has a negative impact on the environment by the alterations of the landscape and the quality of environmental factors. Environmental factors that could be affected by mining operations resulting from exploitation are: water, air, soil, population, fauna, and flora. The aim of this study is to identify and characterize the sources of rocks and soil pollution from natural radionuclides and heavy metals and also to assess the impact on these two environmental factors for an abandoned uranium mining perimeter. The mining exploration and exploitation area chosen as a case study is the Zimbru perimeter, Arad County.

* Corresponding author: daniela_aura_radu@yahoo.com

A STUDY OF THE METHANOL SYNTHESIS PROCESS AT THE LEVEL OF CATALYST PELLET

Ionuț BANU[1*], Ioana STOICA[1], Grigore BOZGA[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

In a fixed bed of porous catalyst pellets, there are developed two composition and temperature fields, one in the fluid phase and the other one inside the catalyst pellets. The limitation effects of mass transport inside a catalyst pellet, on the global kinetics, can be evaluated using mathematical models of different complexities. In the first part of this study, there were compared the process simulation results obtained describing the mass transport inside the pellet by two models, the Dusty Gas model and the simpler Wilke-Bosanquet model. The surface steps kinetics was described by the model published by Graaf et al (1990) and the mass and heat transfer parameters were evaluated by the available literature correlations. In terms of internal effectiveness factor values, the two diffusion models provide practically identical results, this indicating that the frequently used Wilke-Bosanquet model provides an acceptable accuracy.

In the second part of the study, based on the Wilke-Bosanquet model, it was analyzed the process in the catalyst pellet in unsteady state conditions. The calculated response of the pellet to step changes in external composition, evidenced a relatively fast dynamics of the process, characterized by transition times of 3-4 seconds. Also, the response to step changes in external surface temperature (at constant external composition) shown that the stabilization times are about one second shorter than those for composition. The process simulations of non-isothermal process inside the catalyst pellet showed that the internal temperature gradients are practically negligible, in accord with data reported in other studies. Another interesting result is that, for unsteady state pellet operation, the internal effectiveness factor calculated from the unsteady-state mathematical model is well approximated by the one calculated from the steady state equations.

Keywords: methanol synthesis, catalyst pellet, diffusion models, unsteady state regime

_____

[*] Corresponding author: i_banu2003@yahoo.com

SURFACE PROPERTIES OF NOVEL AMINO ACID-BASED AND CARBOHYDRATE-BASED SURFACTANTS

Irina Elena CHICAN[1*], Dana VÂRĂTEANU[1], Loti OPROIU[1], Mircea RUSE[1]

[1]*National Research and Development Institute for Chemistry and and Petrochemistry - ICECHIM Bucharest, 202 Splaiul Independentei, 060021, Bucharest, Romania,*

In surfactant industry there is a trend to replace the surfactants produced from petrochemical feedstocks with surfactants based on renewable raw materials, with positive effect on greenhouse gases emissions. Surfactants with hydrophilic groups consisting of amino acids or carbohydrates and hydrophobic tails from vegetable oils are gaining increased attention due to the high degree of biodegradability and low toxicity [1-4]. In this paper are presented studies regarding the surface active properties of surfactants containing one ore two amino acid or carbohydrate-derived head groups. Surfactants were obtained by processes that comply with the principles of green chemistry (use of the aqueous reaction medium, or if it is not possible use of solvents with low toxicity, reaction temperatures up to 50°C). The surface tension and critical micelle concentration (CMC) in aqueous solutions were determined for 1,l2-digluconamidododecane (bolaform surfactant), lauroyl hydroxyproline, palmitoyl hydroxyproline and 1,12-dodecanedioyl diglycylglycine (bolaform surfactant). Amino acid-based surfactants were saponified with sodium hydroxide solution, ensuring the formation of the active part of the molecule, namely the anion R-COO⁻. The surface tension and CMC were measured with the help of automated tensiometer SIGMA 700 – KSV. Critical micelle concentration is of great importance in determining the optimal concentration for use of surfactants, which is placed at the upper limit of the critical micelle concentration. The influence of the hydrophobic chain length upon CMC was studied for amino acid-based surfactants, also the influence of head groups (one ore two amino acid or carbohydrate-derived head groups). The efficiency of surfactants was evaluated by the difference between the surface tension of distilled water and surface tension at CMC. Efficiency of about 40 mN/m of aqueous solutions of sodium lauroyl hydroxyproline and sodium palmitoyl hydroxyproline, showed that are only slightly less effective in decreasing the surface tension of water at critical micelle concentration compared with sodium dodecyl sulfate (34 mN/m). The study demonstrates that the synthesized surfactants are a viable alternative for the petrochemical compounds.

Keywords: surfactant, amino acid, carbohydrate, critical micelle concentration, surface tension.

---

* Corresponding author: organica@icechim.ro

References

[1] Holmberg K., Natural surfactants, *Curr. Opin. Colloid Interf. Sci*, 6(2), 148-159, 2001.

[2] Clapés P., Infante M.R., Amino Acid-based Surfactants: Enzymatic Synthesis,Properties and Potential Applications, *Biocatal. Biotransf.*, 20(4), 215–233, 2002.

[3] Brito R.O., Silva S.G., Fernandes R.M.F., Marques E.F., Enrique-Borges J., do Vale M.L.C., Enhanced interfacial properties of novel amino acid-derived surfactants: effects of headgroup chemistry and of alkyl chain length and unsaturation, *Colloids Surf. B: Biointerfaces*, 86, 65–70, 2011.

[4] Gatard S., Nasir M. N., Deleu M., Klai N., Legrand V., Bouquillon S*., Bolaamphiphiles Derived from Alkenyl L-Rhamnosides and Alkenyl D-Xylosides: Importance of the Hydrophilic Head*, *Molecules*, vol.18, 6101-6112, 2013.

DETERMINATION OF TRITIUM CONTENTS IN NON-INCINERABLE SAMPLES

Diana CHIPER[1*], C. POSTOLACHE[1], G. BUBUEANU[1]

[1] *"Horia Hulubei" National Institute for Physics and Nuclear Engineering IFIN HH, Magurele, Ilfov, Romania*

In this study, a new facility for determination of tritium content in incinerable and non-incinerable solid wastes is described. The protocol consists of oxidation in two steps of the samples in oxygen atmosphere, HTO kept and determined of T activities at Liquid Scintillation Counting.
Equipment used in experiment is constituted from:
  - Pressure oxygen tub with pressure regulator and flow control Rota meter
  - 2 tube furnace with temperature controller (RT 50-250/11 Nabertherm type), one for sample oxidation and/or calcination (at 200^0C / 400^0C / 900^0C temperatures) and secondary for catalytic oxidation of resulted gases at water and carbon dioxide (700-800^0C in presence of CuO wires catalytic bed)
  - HTO collector
  - Trapping unit for retention of tritiated water over siccative $CaCl_2$
  - Radioactive gas monitor (RGM) with Ionizing Chamber Overhoff type
The equipment was used in the radiological characterization of historical non-incinerable wastes obtained in the refurbishment step of the tritium laboratory.

---

[*] Corresponding author: dchiper@nipne.ro

CONDUCTIVITY CELL CONSTANT REVISITED

Ioana-Alina CIOBOTARU[1*], Florin Mihai BENGA[1], Oana Claudia BARBU[1], George Costin LAZĂR[1], Claudiu CÂMPUREANU[1], Traian RUS, Danuț-Ionel VĂIREANU[1]

[1] *Politehnica University of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Gh. Polizu Street, RO-011061, Bucharest, Romania,*

This paper discusses various problems associated with the determination/calibration of the conductivity cell constant, encountered during the practical evaluation of conductivity in liquids, and attempt to present some conventional and non-conventional solutions (some of them based on novel conductivity probe constructive solutions, which allow an easy modification of the probe configuration and hence the variation of the cell constant) to solve these problems. A procedure for manual temperature compensation, as well as one for replatinising the cell electrodes are also presented.

Keywords: conductivity, cell constant, manual temperature compensation, calibration

References

[1] Shreiner R.H., Pratt K.W., Standard Reference Materials: Primary Standards and Standard Reference Materials for Electrolytic Conductivity, National Institute of Standards and Technology, Special Publication 260-142, Gaithersburg, 2004.
[2] Vaireanu D.I., *Handbook of Experimental Electrochemistry*, Ed. Printech, Bucharest, ch 2, 2008.
[3] Vaireanu D.I., Maior I., Grigore A, Săvoiu D., The evaluation of ionic conductivity in polymer electrolyte membranes, *Rev. Chimie*, 59, 10, 1140-1142, 2008.
[4] Vaireanu D.I., Cojocaru A., Maior I., Caprarescu S., Practical considerations regarding the measurement of ionic conductivity by EIS in conductive polymers, *Chem. Bull. "POLITEHNICA" Univ. of Timisoara, Series Chemistry and Environmental Engineering*, 1-2, 258-261, 2008.
[5] Caprarescu S., Vaireanu D.I., Cojocaru A., Maior I., Purcar V., A 3-cell electrodialysis system for the removal of copper ions from electroplating wastewater, *Optoelectronics and Advanced Materials – Rapid Communications*, 12, 1346-1351, 2011.
[6] Deszo D., *Electrokemiai Tablazatok*, Ed. Musyaki Konzvkiado, Budapest, ch 2, 1965.
[7] Ciobotaru I.A., Maior I., Cojocaru A., Caprarescu S., Vaireanu D.I., Ciobotaru I.E., The determination of the optimum hydrolysis time for silane films deposition, *Applied Surface Science*, 371, 275-280, 2016.

---
[*] Corresponding author: ioanaalinaciobotaru@yahoo.com

AN EXPERIMENTAL INVESTIGATION ON THE DYNAMIC VISCOSITIES OF ALGAL SUSPENSIONS

Doini a-Roxana CIOROIU[1*], Oana Cristina PÂRVULESCU [1], Rodica ANGHEL[1], Claudia Irina KONCSAG[2], T nase DOBRE[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[2] *Ovidius University of Constanta, 124 Mamaia Street, Constanta, 900527, Romania*

Seaweeds from coastal waters of the Black Sea (Ceramium rubrum, Cladophora vagabunda, Ulva lactuca and Cystoseira barbata) represent an important renewable source of energy which can be the answer for biofuels demand. Experimental study on the dynamic viscosities of aquatic macrophytes aim to predict the flow of fluids in the equipment for fuel manufacture. In this work, we perform a rheological study of fluids prone to take part in the processes. In the solid-liquid extraction from algae, these are finely ground to achieve the conditions for reducing resistance to transport and transfer of extracted components through the liquid phase. Then aqueous suspensions are obtained from each species of above mentioned algae, so we made three algal suspension of different concentrations: 5%, 10% and 15%. The samples were mixed well, kept for about 2 hours at 25°C and analyzed with the rotational viscometer Rheotest-2, then correlating the sample volume with the type of the cylinder.

Dynamic viscosity measures the dependence on shear rate on the shear stress. The apparent viscosity of suspension were calculated and, as expected, the more diluted suspensions were less viscous (0.02-0.08 Pa s) and the more concentrated suspensions had viscosities between 0.08-15.77 Pa s. The non-newtonian behaviour of these suspensions is also discussed in the paper.

These measurements are important for the calculation of power consumed in the stirrer system of the extractors with mechanically agitation used to separate some compounds of interest from algae. Also, it is important to know the viscosity values for mass transfer calculations where they intervene in Schmidt numbers determination (Sc).

Keywords: algae, aqueous suspensions, dynamic viscosity.

Reference
[1] Vassilev S.V., Vassileva C.G., Composition, properties and challenges of algae biomass for biofuel application: An overview, *Fuel*, Volume 181, 1-33, 2016.
[2] León-Martínez F.M., Cano-Barrita P.F. de J., Lagunez-Rivera L., Medina-Torres L., Study of nopal mucilage and marine brown algae extract as viscosity-enhancing admixtures for cement based materials, Construction and Building Materials, Volume 53, 190-202, 2014.

---

* Corresponding author: roxana.cioroiu@yahoo.com

EFFICIENCY OF NATURAL WOOL FIBERS (NWF) IN OIL SPILL CLEANUP

Alina-Georgiana CIUFU[1*], Dobre TANASE[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Remediation of oil spills in open waters is a research topic of great importance. The need to find the most efficient sorbent for the clean-up of oil spills both at sea and land is of an extreme importance. Natural oil sorbents (e. g. cotton, cork, peat moss, straw) are among the alternatives for oil removal from the marine ecosystem. Although, two major problems of many natural oil sorbents are low hydrophobicity and low buoyancy. Natural wool fibers with their excellent oil removal properties, hydrophobicity, environmental friendliness, buoyancy and availability are an attractive alternative for accidental oil spills.

This study it's focused on the natural wool fibers for the removal of various pollutants, such as: crude oil (three types: Basrah, Azeri and Crude Oil), diesel fuel, gasoline and mixture of 50 % gasoline and 50% diesel fuel from the marine environment. Sorption capacity of the sorbent in water and in oil without water, oil retention, sorbent reusability, buoyancy in static and dynamic conditions and contact angle were investigated. Efficiency of oil removal was determined by measuring the oil concentration before and after the sorption process. The measured contact angles suggest that wool is hydrophobic (water 118.32 +/- 3.68) and oleophilic – two key properties of a good sorbent. The factors for sorbent efficiency were analyzed. The results presented and discussed in this work show that sorption process is mostly affected by sorption time, mass of sorbent, pH value of water and temperature.

Oil-sorbent wool products are light and easy to transport, they have good oil sorption properties (it can absorb 10 to 30 times its weight in oil while repelling water, making it significantly more efficient as oil absorbent than polypropylene) like: hydrophobicity, excellent reusability (it can be wrung out and reused), biodegradability, good buoyancy, which make wool – based sorbents a viable alternative to commercially available synthetic sorbents and could be used for removal of oil from water.

Key words: Sorption capacity, Oil retention, Natural Sorbent, Buoyancy, Hydrophobicity

---

[*] Corresponding author: alinag.ciufu@gmail.com

ELECTRODE PROCESSES DURING SeTe AND PbSeTe FILM FORMATION USING DEEP EUTECTIC SOLVENTS BASED ON CHOLINE CHLORIDE

Ion SIN[1], Anca COJOCARU[1*], Liana ANICAI[2], Adina COTÂRȚĂ[1], Teodor VIȘAN[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*
[2] *Center of Surface Science and Nanotechnology, University POLITEHNICA Bucharest, Romania*

The aim of this work is to study the electrode processes during electrolysis in two ionic liquids based on choline chloride (ChCl), namely ChCl-urea and ChCl-ethylene glycol, with the advantage of a high-electrochemical window of such deep eutectic systems. We report here an investigation of electrodeposition of singular Se, Te and Pb elements, as well as codeposition of their binary and ternary semiconductor compounds. Cyclic voltammograms (CVs, with 5-100 mVs^{-1} scan rates) and electrochemical impedance (EIS) spectra (ac frequency between 100 kHz and 50 mHz) were recorded using the SP150 Bio-Logic Sci. Instr. potentiostat. The precursors were SeO_2, TeO_2 and $PbCl_2$, respectively, and the working electrode was a Pt plate (0.5 cm^2).

CV curves recorded from electrolytes containing single lead ion have shown the couple of deposition/stripping dissolution of Pb metal. In the voltammograms for electrolytes with single Se^{4+} or Te^{4+} ions, successive processes of underpotential deposition, bulk deposition and further conversion of solid deposit into a soluble species (Se^{2-} or Te^{2-}) appeared by gradual scanning toward negative values. CVs regarding the deposition of binary (SeTe, PbSe, PbTe) and ternary (PbSeTe) compounds showed clearly a corresponding cathodic peak. EIS spectra as Nyquist plots showed a series of semicircles with the diameter decreasing by more negative potential polarization; in some cases they are continued with a straight line (a tail) at lower frequencies indicating the film deposition. The maximum phase angles in Bode plots also showed relatively high values of phase angle (from -50 to -70°) that correspond to semiconductor behavior of films, but decreased phase angle (cca. -30°) was registered for PbSeTe compound.

Keywords: ionic liquids, electrodeposition of Se, Te, Pb, SeTe and PbSeTe films

References

[1] He B., Zhang W., *II-VI Semiconductors and their device applications* (chapter 11.4), in: F. Devillanova, W.W. Du Mont (Eds), *Handbook of Chalcogen Chemistry: New Perspectives in Sulfur, Selenium and Tellurium*, Vol. 2, 2nd edition, RSC Publ., Cambridge, 2013, 180.

[2] Abdel Aal A., Voigts F., Chakarov D., Endres F., Electrodeposition of selenium from 1-butyl-1-methylpyrrolidinium trifluoromethylsulfonate, *Electrochim. Acta*, 59, 228-236, 2012.

---

* Corresponding author: anca.cojocaru@chimie.upb.ro

[3] Cojocaru A., Sima M., Electrochemical investigation of the deposition/dissolution of selenium in choline chloride with urea or ethylene glycol ionic liquids, *Rev. Chim.* (Bucharest), 63, 217–223, 2012.

[4] Abdel Aal A., Voigts F., Chakarov D., Endres F., Electrodeposition of selenium from 1-ethyl-3-methyl-imidazolium trifluromethylsulfonate**,** *J. Solid State Electrochem.*, 16, 9, 3027-3036, 2012.

[5] Cojocaru A., Sin I., Agapescu C., Cotarta A., Visan T., Electrode Processes and SEM/EDX Analysis of Selenium Films Electrodeposited From Ionic Liquids Based on Choline Chloride, *Chalcogenide Letters*, 13, 3, 127-138, 2016.

MATHEMATICAL SIMULATION OF COMPOUNDS' SEPARATION BY SOLID PHASE EXTRACTION USING SELECTIVE ADSORBENTS

Ştefan-Ovidiu DIMA[1,2*], Tănase DOBRE[1]

[1]*University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*
[2]*INCDCP-ICECHIM, Bioresources Department, 202 Splaiul Independentei, 060021 Bucharest, Romania*

The mathematical model used in this work to simulate the separation of various compounds from complex mixtures, like extracts from agro-resources and biomass, is an up-grade of a mathematical model designed for the study of adsorption-desorption processes that take place in a fixed bed of selective polymer pearls obtained by molecular imprinting [1].

Molecularly imprinted polymers (MIPs) are selective materials designed to have increased affinity for a target molecule or a class of compounds, being known also as artificial antibodies due to the principle by which they gain their selectivity in the presence of the target molecule, similar with the antigen-antibody interactions [2-4]. Their high selectivity is the reason why their application area is extremely vast and in continuous expansion, ranging from pharmaceutical industry, biomedical science, engineering, sensors and biosensors, environment protection, analytical applications and others [3,4]. In brief, a MIP is a polymer which is designed to be selective for a target molecule called template by a reverse lock & key mechanism, meaning the lock is build around the key aiming to include as much as possible from the key pattern in order to increase the lock's affinity [1,2].

Regarding the adsorption in MIP pearls, the experimental studies suggested that the initial hypothesis of linear adsorption is a significant approximation that requires improvement. The present study is investigating two new hypotheses regarding the type of selective adsorption in molecularly imprinted polymers, meaning the adsorption after power law and, additionally, after a hyperbolic law. The adsorption dynamics data were described with the help of a phenomenological mathematical model that has as main parameters the adsorption coefficient - k_a, the desorption coefficient - k_d, and the coefficient of effective diffusion - D_{ef}. The parameters' identification evidenced a slowly dependence of these parameters on the adsorbed target molecule concentration, and a heavier influence of the type of copolymer that is used to build the MIP matrix.

Keywords: mathematical modelling, solid phase extraction, selective adsorbents, molecularly imprinted polymers, MIPs.

---

* Correspondin author: phd.ovidiu.dima@gmail.com

References
[1] Dima S.O., Dobre T., Mathematical modeling and simulation of adsorption process in a fixed bed of molecularly imprinted polymeric pearls, *UPB Sci. Bull. B*, 78 (2), 143-154, 2016.
[2] Dima S.O., Nicolae C.A., Iordache T.V., Chetraru O., Meouche W., Faraon V.A., Donescu D., Thermal analyses as tools for proving the molecular imprinting with diosgenin and sclareol in acrylic copolymer matrices, *J. Therm. Anal. Calorim.*, 120 (2), 1107-1118, 2015.
[3] Zheng H.Y., Yoshikawa M., Molecularly imprinted cellulose membranes for pervaporation separation of xylene isomers, *J. Membr. Sci.*, 478, 148-154, 2015.
[4] Bedwell T.S., Whitcombe M.J., Analytical applications of MIPs in diagnostic assays: future perspectives, *Anal. Bioanal. Chem.*, 408 (7), 1735-1751, 2016.

PHYTOTOXICITY TESTS OF SEEDS ON RADIOACTIVE CONTAMINATED SOILS

Oana DOBRE[1*], Alexandru WOINAROSCHY[2], Eugenia PANȚURU[1]

[1] *Research & Development National Institute for Metals and Radioactive Resources, 70 Carol I Bvd., 020917, Bucharest, Romania*

[2] *University "Politehnica" of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Str. 011061, building L, Bucharest, Romania*

In the present paper was studied the influence of uranium toxicity, on seed germination and root elongation of three types of seeds: alfalfa (Medicago sativa), cress (Lepidium sativum) and turf. Experiments were performed using solutions with different uranium concentrations compared to a reference sample - distilled water, respectively: 6 ppm; 12ppm; 25 ppm; 50 ppm; 75 ppm and 150 ppm. The experimental results showed that germination and root elongation decreased with increasing uranium content in soil.

Keywords: Phytoremediation, contaminated soils, uranium

---

* Corresponding author: spirache_oana@yahoo.com

ON CONVEYOR DRYING OF POROUS GYPSUM BOARDS

Oana PÂRVULESCU[1], T nase Gh. DOBRE[1*], Diana MATEI[1]

[1] University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania

A mathematical model for drying of porous flat slabs on a conveyor belt has been developed. The model considers the coupled moisture and heat balance equations when the water flow rate exiting from a pore of the material follows a diffusion process through a stagnant gas layer. The pore diameter, pore tortuosity, slab porosity, drying air relative humidity and belt velocity were selected as process factors. At the slab surface, where the air flows tangentially, the model considers: (i) no mass and heat transfer resistance; (ii) mass transfer resistance and no heat transfer resistance; (iii) heat and mass transfer resistance. The gypsum board drying was selected as case study. In the first modeling case it is assumed that the air and gypsum board have the same temperature, the mass transfer resistance at the board surface is negligible and the air humidity remains constant due to a high value of its flow rate. The model solution is an analytical expression for mean moisture content of the board, which emphasizes that air temperature, air humidity, belt velocity and the board position on the conveyor belt control the drying process. In the second modeling case the mass transfer resistance is taken into account. Depending on dynamics of air humidity, two situations appear in this case. For a high value of air flow rate, the model solution is a differential equation showing the state of mean moisture content of gypsum board depending on its position on the conveyor belt. For a moderate value of the air flow rate, the air humidity is variable along the conveyor belt and the differential equation characterizing the board moisture content is coupled with the differential equation for local air humidity in the device. Characteristic mathematical model of the third case consists of four differential equations referring to board mean moisture content and temperature, air humidity and temperature.

Keywords: gypsum board, mean humidity, mass transfer, heat transfer, mathematical modeling

---

[*] Corresponding author: tghdobre@gmail.com

SIMULATION OF THE CONTROLLED RELEASE OF DRUGS FROM POLYMERIC DOSAGE FORMS: A CASE STUDY

Paula POSTELNICESCU[1], Anca Mădălina DUMITRESCU[1*], Roxana NEGRU[1], Diana NEGRU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

The aim of controlling the drug delivery is to achieve more effective therapies while eliminating potential for both under- and overdosing.

The controlled release dosage form is required to improve the bioavailability of drug and the patient compliance by modifying the rate of drug absorption which reduces the frequency of dosing.

Over the past three decades, because the oral dosage forms are generally made of polymers in which the drug is dispersed, the controlled release from a polymeric matrix was a problem of special interest in the area of pharmacokinetics.

Because many mathematical models were developed to describe the release of drugs from oral dosage forms, it is very important to identify an adequate model for a specific drug delivery system.

The choice of an appropriate model depends on the type of drug, type of excipients and composition of the dosage form.

This paper presents the results of a kinetic study regarding the controlled release of cefixime, a third generation oral cephalosporin, from different polymeric matrixes. In order to illustrate the validity of the selected models, comparisons with experimental profiles obtained in simulated intestinal fluid (pH 7.4) and reported in the recent literature are presented. The predictions of the mathematical models are useful to improve the oral administration of the considered antibiotic.

Keywords: drug delivery, controlled release, polymeric matrix

---

[*] Corresponding author: a_dumitrescu@chim.upb.ro

PREPARATION AND CHARACTERIZATION OF Al(III)-PILLARED INTERLAYERED CLAYS BASED ON INDIGENOUS BENTONITE

Ana-Maria GEORGESCU[1*], Vasilica Alisa ARU [1], Françoise NARDOU[2], Ileana Denisa NISTOR[1]

[1] *"Vasile Alecsandri" University of Bacău, Faculty of Engineering, Chemical and Food Engineering Department, 157 Calea Marasesti Street, 600115 Bacau, Romania*
[2] *University of Limoges / CEC, SPCTS, UMR 7315 CNRS, 12 Rue Atlantis, 87068 Limoges Cedex, France*

Al-pillared interlayered clays (Al-PILCs) were prepared from Romanian natural calcium bentonite (Orasu Nou deposit) and the effect of some parameters on the textural properties has been investigated. The synthesis of Al-pillared bentonite consists in the following steps: bentonite purification, ionic exchange of bentonite with Cu(II) ions, preparation of pillaring agent, intercalation of ionic exchanged bentonite with pillaring agent and calcination.

The synthesized nanomaterials were characterized by X-ray diffraction (DRX) analysis, nitrogen adsorption-desorption technique for the measurement of specific surface area by using of BET method (Brunauer - Emmet - Teller) and the pore size distribution by using the BJH method (Barrett - Joyner -Halenda). The basal spacing, specific surface area and pore size distribution were strongly affected by the varied parameters.

The material with the best textural characteristics will be chosen in the aim of its using in environmental remediation.

Keywords: bentonite, basal spacing, specific surface area, porosity

---

[*] Corresponding author: ana.georgescu@ub.ro

OBTAINING OF MOLECULARLY IMPRINTED FILMS VIA ELECTROPOLYMERIZATION BASED ON [TETRAKIS(2,2'-BITHIOPHENE-5-YL)SILANE] MONOMER

Elena-Bianca GEORGESCU[1*], Hugues BRISSET[2], Catherine BRANGER[2], Ana-Mihaela FLOREA[1], Tan a-Verona IORDACHE[1], Anita-Laura RADU[1], Catalina-Paula SP T RELU[1], Andrei SÂRBU[1]

[1] *National Research and Development Institute for Chemistry and Petrochemistry ICECHIM, Bucharest, Romania*

[2] *University of Toulon-Var, MAPIEM Laboratory, La Garde, France*

The illicit transport of drugs is a big problem all over the world. This directly affects people health and the quality of life. In addition, the increase of drug derivates to be monitored requires more suitable analytical methods. Molecularly imprinted polymers (MIPs) are recognition elements capable to recognize a large variety of target structures with antibody-like affinities and selectivity. Conducting polymers based on thiophene or pyrrole are attracting attention as organic materials for electrochemical sensors due to a combination of properties. Monomers are easy to functionalize, and depending upon the functional groups and chain architecture, these polymers are used since three decades to prepare modified electrodes to develop sensors [1]. Optical sensors represent a group of chemical sensing receptors in which electromagnetic radiation is used to generate the analytical signal in a transduction element. The interaction of this radiation with the sample is evaluated from the change of particular parameter and is related to the concentration of the analyte [2].

Herein, we report the preparation of tetrakis(2,2'-bithiophene-5-yl)silane monomer which was further used to obtain polymer films via electrochemical procedures. LC-MC and XRD (figure 1) were used for monomer analysis.
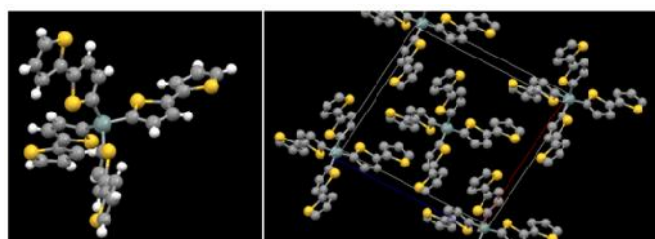
Figure 1. XRD – analysis of tetrakis(2,2'-bithiophene-5-yl)silane

Polymer films were obtained by electropolymerization in presence of a template molecule using electrolyte solution.

---

[*] Corresponding author: georgescu_elena_bianca@yahoo.com
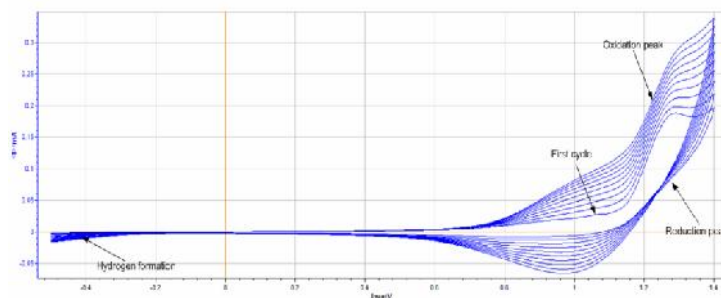
Figure 2. MIP –electropolymerization: multiple scans -0.5– 1.4 V in 0.1 M ACN/TBAPF$_6$, rate scan 100 mV/s

Keywords: MIP, sensor, electropolymerization, template, silane.

References
[1] Gründler P., *Chemical Sensors, An Introduction for Scientists and Engineers*, Springer-Verlag, Berlin Heidelberg, 2007.
[2] Lukowiak A., Sterk W., Sensing abilities of materials prepared by sol-gel tehnology, *J.Sol-Gel Sci Technol.*, 50, 201-2015, 2009.

SIMULATION OF PROCESS TO CONCENTRATE HEMP OIL METHYL ESTERS

Elena-Bianca GEORGESCU[1,2*], Petrica IANCU[2], Valentin PLEŞU[2], Nicoleta-Gabriela ŞTEFAN[2]

[1] *National Research and Development Institute for Chemistry and Petrochemistry ICECHIM, Bucharest, RO*

[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Omega-3 and omega-6 are recommended for a normal diet due to their positive effects on human health. These acids are not produced by human body, thus they need to be synthetized from different natural sources. Hemp oil is rich in omega-6 (linoleic acid) and omega-3 (linolenic acid) [1]. Transesterification reaction is the classical procedure for obtaining methyl esters. Before distillation is necessary to calculate critical properties (normal boiling point, critical temperature, critical volume etc).

Vacuum distillation was used for separation and concentration of obtained methyl esters. After two separation steps, both distillate and bottom phases were analyzed by gas chromatography and was observed that the methyl linoleate concentration was increased to 62%. For experimental part was used DSL-5 plant – vacuum distillation plant [2].

The methyl esters concentration process from hemp oil is complex due to the nature of gliceride and esters molecule. This process was simulated in ASPEN Plus using thermodinamics properties calculated by group contribution. For conceptual process design were identified two blocks: reaction block and separation block. Reaction block is composed by transesterification reactor and separation block contain the purification of methyl esters part and glycerol recovery part. For separtion block, two separation columns, under vaccum conditions were used. After purification, methyl linoleate concentration obtained in the simulation programe was 59% (wt) compared with 62%(wt) obtained by experimental procedure.

Keywords: hemp, esters, transesterification, distillation, concentrate.

---

[*] Corresponding author: georgescu_elena_bianca@yahoo.com

References

[1] Ragit S.S., Mohapatra S.K., Gill P., Kundu K., Brown hemp methyl ester: Transesterification process and evaluation of fuel properties, *Biomass and Bioenergy*, 41, 14-20, 2012.

[2] Stefan N.G, Plesu V., Iancu P., Georgescu E.B., New possibilities to obtain concentrates of PUFA esters by high vacuum distillation*, 3th European Congress of Applied Biotehnology*, Nice, France, 27 September – 1 October 2015.

PHYSICO-CHEMICAL BEHAVIOR ON GLYCINE DERIVED COMPOUNDS IN AQUEOUS D-GLUCOSE SOLUTIONS AT DIFFERENT TEMPERATURES

Florinela SIRBU[1*], Ioana GHEORGHE[1], Amalia STEFANIU[2], Cristina STOICESCU[1], Valeria Gabriela SAVOIU[2]

[1] *Institute of Physical Chemistry Ilie Murgulescu of the Romanian Academy, Bucharest, Romania*

[2] *National Institute for Chemical - Pharmaceutical Research and Development - Bucharest, 112 Vitan Av., 031299, Bucharest, Romania*

The objective of this study was to carry out an analysis on physico-chemical behavior of glycine, and N-Methylglycine, respectively, in aqueous D-glucose solutions.

Densities, speed of sound, and refractive index of glycine, and N-Methylglycine in aqueous D-glucose mixtures were measured over the whole composition range for amino acids between (0.1 and 1) $mol \cdot dm^{-3}$ in 0.4 $mol \cdot dm^{-3}$ of D-glucose at different temperatures of (308.15 and 318.15) K and at atmospheric pressure. Using the experimental data obtained the derived thermophysical properties as apparent molar volumes, isentropic compressibility, and molar refractivity were calculated. The refractive indices values have been computed using Lorentz-Lorentz equation.

The standard partial molar volumes, standard partial molar volumes of transfer and hydration numbers for the amino acids were also determined.

The influence of the aminoacid composition and carbohydrate concentration on the thermophysical properties has been evidenced. The obtained results have been interpreted in terms of solute-cosolute and solute-solvent interactions present in these studied ternary aqueous mixtures.

Keywords: Physico-chemical properties; Glycine; N-Methylglycine, D-glucose solutions, ternary mixtures

References
[1] Nain A. K., Pal R., Study of solute–solute and solute–solvent interactions of l-threonine in aqueous-glucose solutions at different temperatures by using volumetric and viscometric methods, *J. Chem. Thermodyn.*, 60, 98-104, 2013.
[2] Gheorghe I., Stoicescu C., Sirbu F., Partial molar volumes, isentropic compressibilities, and partial molar expansibilities of N-Methylglycine and d-Glucose in aqueous environments at temperatures between (298.15 and 323.15) K, *Journal of Molecular Liquids*, 218, 515-524, 2016.

* Corresponding author: sflorinela@yahoo.com

RADIATIVE TRANSFER APPROACH FOR ACTINOMETRY IN SIMPLE AND COMPLEX GEOMETRIES

V. ROCHATTE[1,2], G. DAHI[1,2], A. ESKANDARI[1,2], J. DAUCHET[3,2], Fabrice GROS[3,2*], M. ROUDET[3,2], J.-F. CORNET[3,2]

[1] *Université Clermont Auvergne, Université Blaise Pascal, Institut Pascal, BP 10448, F-63000 Clermont-Ferrand, France*

[2] *CNRS, UMR 6602, IP, F-63178 Aubière, France*

[3] *Université Clermont Auvergne, SIGMA Clermont, Institut Pascal, BP 10448, F-63000 Clermont-Ferrand, France*

Among all the parameters studied in the engineering photoreactive systems, estimating the photon flux density, q, entering the environment is of primary importance as this parameter is the basis of any study and any analysis of a photoprocess. To estimate this value, different physical means of local measurement are available, such as photodetectors, bolometers. Besides these instruments, chemical actinometers such as ferrioxalate are also widely used. These molecules undergo a chemical reaction under the effect of light with a specific quantum efficiency of known value. The kinetics of the actinometer decomposition can be experimentally measured, a widespread simplified model only valid in specific conditions, allows the determination of the average photon flux entering the reactor. Indeed the operating conditions traditionally encountered in the literature (high optical thickness, low conversion rate) help to ensure that all photons which enter the solution are absorbed by the actinometer. This implies a linear evolution of the concentration of reaction products in the system directly proportional to q.

In this work, we present a complete radiative transfer approach for estimating incident photon flux density by actinometry that will open the door to the investigation of large-scale intensified photoreactors. Our methodology is based on the original concept of the analysis of the probability that a photon entering the reaction volume is absorbed by the actinometer. This probability is usually assumed to be equal to one in classical actinometry, facilitating the identification of photon flux density as already explained. However, such an assumption can no longer be satisfied in many practical situations in which optical thicknesses are low.

Hence this restriction is removed by using most recent advances in the field of radiative transfer Monte Carlo, in order to rigorously evaluate the instantaneous absorption-probability as a function of conversion. Implementation is performed in EDStar, an open-source development environment that enables straightforward simulation of reactors with any geometry (directly provided by their CAD-file), with the very same Monte Carlo algorithm.

Experimental investigations are focused on the Reinecke's salt photodissociation in two reactors designed for the study of natural and artificial photosynthesis. The first reactor investigated serves as reference configuration: its simple 1D torus geometry allows to compare flux densities measured with quantum sensors and actinometry. Validations and analysis are successfully carried out on this reactor. Then, the approach is

---

implemented on a 25 L photobioreactor with complex geometry corresponding to one thousand light-diffusing optical fibers distributing incident photons within the reaction volume. Besides evidence of high reproducibility of the experiments, results and models show that classical actinometry neglecting radiative transfer can lead to 50 percent error when measuring incident flux density for such reactors. However the emission angular distribution (collimated or lambertian emission) couldn't have been determined.

Finally, we propose how this radiative transfer approach paves the way for analyzing high conversion as a mean to investigate angular distribution of incident photons, provided a suitable actinometer may be developed.

APPLICATION OF CORRELATION ALGORITHMS ON MONITORING DATA FOR QUALITY ASSESSMENT OF THE AQUATICECOSYSTEMS

Petra IONESCU[1*], Alexandru Anton IVANOV[1], Elena DIACU[2], György DEÁK[1]

[1] *National Institute for Research & Development in Environmental Protection, Spl. Independentei, 294, 6th District, Code 060031, Bucharest, Romania*

[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

At a global level, water pollution represents a critical problem, so the proper management of water resources involves continuous monitoring of its quality. The multitudes of data from monitoring programs require the use of indices and algorithms for evaluating water quality as suggestive as possible. Developing sets of indices and ecological indicators is a priority at European level.

This paper aims to assess the surface water quality in relation to the heavy metal content according to national regulations by a modern approach of data processing from monitoring programs. To achieve the propose, a data set obtained from a monitoring program conducted during January-April 2015 under the contract 53/2015 entitled "Monitoring of environmental impact of the works for improvement of navigation conditions on the Danube between C l ra i and Br ila, km 375 and km 175" has been used, and the following data correlation algorithm have been developed and applied: Heavy metal Pollution Index, Metal Index and Multi-Parametric Quality Index applied to metal concentrations.

The Heavy Metal Pollution index has been an effective tool for assessing the level of pollution of surface waters in terms of heavy metal content providing information on the influence of each metal in particular to the overall water pollution. The application of Metal Index on monthly average values has led to the classification of the Lower Danube as water quality class II (good) according to regulations. With the purpose of intercomparison to other indices and to the general indices of ecosystem quality focused on indicators values of heavy metals class, a smaller version of the ICPM algorithm has been analyzed, considering all the heavy metal values. The ICPM values (metals) ranged from 33% to 38% except for March that was higher, up to 68%.

Keywords: Heavy Metal Pollution Index, Metal Index, Multi-Parametric Quality Index, aquatic ecosystem

References

[1] Contract nr. 6N/februarie 2009, act adi ional nr. 2/2015 - PN 09 06 02 39, *Fundametarea ştiinţifică a algoritmilor de evaluare a intercondiţionărilor reciproce dintre capacitatea suport a ecosistemelor acvatice şi elementele de ordin abiotic determinate la nivel de ape de suprafaţă* (INCDPM, Bucure ti).

---

[*] Corresponding author: petraionescu2012@yahoo.ro

[2] Contract nr. 53/2011, *Monitorizarea impactului asupra mediului a lucrărilor de îmbunătăţire a condiţiilor de navigaţie pe Dunăre între Călăraşi şi Brăila, km 375 - km 175* (INCDPM, Bucure ti).

[3] Radu V.-M., Ivanov A.A., Ionescu P., Deák Gy., Diacu E., Overall assessment of water quality on Lower Danube River using multi-parametric quality index, *Rev. Chim.* (Buchrest), vol. 67, no. 3, 391-395, 2016.

MULTIVARIATE STATICS TOOLS USED FOR ROMANIAN HONEY CLASSIFICATION

Raluca Daniela ISOPESCU[1*], Ana Maria JOSCEANU[2], Teodora COLTA[3], Roxana SPULBER[3]

[1]*University Politehnica of Bucharest, Department of Chemical and Biochemical Engineering*

[2]*University Politehnica of Bucharest, Department of Analytical Chemistry and Environmental Protection*

[3]*Beekeeping Research and Development Institute, 42 Ficusului Avn., sector 1, Bucharest, Romania*

The use of complex statistical tools is of great interest when certain products are characterised by a relatively large number measured variables. The appreciation of food quality is always a multivariate problem, as several characteristics must be measured and considered when validating a certain product. Classification procedures, called also pattern recognition methods, are used to characterize groups of samples. Sample measurements may be used to classify samples according to their origin, to distinguish normal and abnormal products or to detect adulteration.

Exporting approximately 8000 tons per year of linden, acacia, sunflower, and colza honey, Romania contributes to the European market with significant amounts of unifloral and polyfloral honey of remarkable good quality. Given the high value of the product, any attempt to modify the natural composition can be classified as adulteration. A large number of data available at APIMONDIA testing laboratories may be used for honey classification according to botanical and geographical origin. These data are obtained for honey sample provided by individual beekeepers and labelled according to their own declarations. For all samples the main characteristics are registered together with information about the period and site of collection. Several multivariate procedures (Principal Component Analysis, Linear Discriminant Analysis, Neural Network Recognition tools) are used to identify the main honey properties that differentiate several honey types and form classes according to botanic and/or geographic origin.

The mathematical tools created can be used in identifying some unknown samples or put into evidence samples that are outliers and should be re-evaluated if some adulteration is possible.

Keywords: multivariate statics, honey, classification

---

* Corresponding author: r_isopescu@chim.upb.ro

PREPARATION AND CHARACTERIZATION OF NEW COMPOSITE MEMBRANES CONTAINING POLYVINYLPYRROLIDONE, POLYVINYL ALCOHOL, SULFOSUCCINIC ACID, SILICOTUNGSTIC ACID AND SILICA FOR DIRECT METHANOL FUEL CELL APPLICATIONS

Said MAAROUF[1,2*], Bouchra TAZI[1*], Farhat GUENOUN[2]

[1]*Laboratoire de chimie biologie appliquée à l'environnement. Faculté des Sciences, Université Moulay Ismail BP :11201 Zitoune Mèknès Maroc*
[2]*Laboratoire de Chimie, DSB, Ecole Nationale d'agriculture de Meknès, BP:S/40Meknes Maroc.*

A novel ionic polymer membranes of different thicknesses (50-450μm) based on polyvinylpyrolidone (PVP), polyvinyl alcohol (PVA), sulfosuccinic acid, and silicotungstic acid (SiWA) with or without silica have been synthetized for polymer electrolyte membrane fuel cells (PEMFCs). The chemical characterization of the membranes has been studied by Fourrier Transform Infrared Spectroscopy (FT-IR). The thermal stability of the membranes has been studied using the techniques of thermogravimetric analysis (TGA) and differential thermal analysis (DTA) between room temperature and 600°C. The water uptake, ionic conductivity, ionic exchange capacity, and fixed ion concentration of these membranes were determined. Water uptake of these membranes ranged between 30% to 75%. The ionic conductivities of these membranes ranged between $1.02 \cdot 10^{-3}$ S/cm to $7,32 \cdot 10^{-3}$ S/cm. The best water uptake and ionic conductivity were those of the membrane based on PVA, PVP, SSA, 10.30 wt.% of SiWA and 5.15wt% of Silica .Whereas the highest ion exchange capacity was 3.79 mmol/g.

Keywords: Polymer electrolyte membranes, Polyvinylpyrrolidone, Polyvinyl alcohol, Sulfosuccinic acid, silicotungstic acid, Ionic conductivity, Fuel cell.

---

* Corresponding author: saidmaarouf576@gmail.com

SYNTHESIS AND CHARACTERIZATION OF NEW COMPOSITE MEMBRANES BASED ON POLYVINYLPYRROLIDONE, POLYVINYL ALCOHOL, SULFOSUCCINIC ACID, PHOSPHOMOLYBDIC ACID AND SILICA

Said MAAROUF[1,2], Bouchra TAZI[1*], Farhat GUENOUN[2]

[1]*Laboratoire de chimie biologie appliquée à l'environnement. Faculté des Sciences, Université Moulay Ismail, BP :11201 Zitoune Meknès Maroc*

[2] *Laboratoire de Chimie, DSB, Ecole Nationale d'agriculture de Meknès, BP:S/40 Meknès Maroc.*

Several new composite proton conducting polymer membranes of different thicknesses (50-500µm) based on polyvinylpyrolidone (PVP), polyvinyl alcohol (PVA), sulfosuccinic acid (SSA) and phosphomolybdic acid (PMA) with or without silica have been developed for polymer electrolyte membrane fuel cells (PEMFCs). The chemical characterization of the membranes has been studied by Fourrier Transform Infrared Spectroscopy (FT-IR). The thermal stability of the membranes has been studied using the techniques of thermogravimetric analysis (TGA) and differential thermal analysis (DTA) between room temperature and 600°C. The water uptake, ionic conductivity, ionic exchange capacity and fixed ion concentration of these membranes were determined. Water uptake of these membranes ranged between 25% to 93%. The ionic conductivities of these membranes ranged between $4,65 \cdot 10^{-3}$ S/cm to $1.33 \cdot 10^{-2}$ S/cm. The best water uptake and ionic conductivity were those of the membrane PVA-SSA-PVP-18.10PMA-7.69SiO$_2$ based on 45.25 wt% of PVA, 10.86 wt% of SSA, 18.1 wt% PVP, 18.1 wt% PMA and 7.69 wt% SiO$_2$ and the membrane PVA-SSA-PVP-19,61PMA containing 49.02 wt% of PVA, 11.76 wt% of SSA, 19.61 wt% PVP and 19.61 wt % of PMA. The membrane PVA-SSA-PVP-19,61PMA gave ionic conductivity of about $4.65 \ 10^{-3}$ S/cm in 1M NaCl media and $4,95 \cdot 10^{-3}$ S/cm in 1M H$_2$SO$_4$ media. The membrane PVA-SSA-PVP-18.10PMA-7.69SiO$_2$ gave ionic conductivity of about $8.07 \ 10^{-3}$ S/cm in 1M NaCl media and reach $1.35 \cdot 10^{-2}$ S/cm in 1M H$_2$SO$_4$ media. The ion exchange capacity of the PVA-SSA-PVP-19.61PMA and PVA-SSA-PVP-18.10PMA-7.69SiO$_2$ membranes were 2.92 and 3.79 mmol/g respectively.

---

* Corresponding author: saidmaarouf576@gmail.com

STUDY OF RADIOACTIVITY SUPERPOSITION / CUMULATION OF POTENTIAL POLLUTANT RADIOISOTOPES DISCHARGED INTO THE ENVIRONMENT

Simona-Eugenia MANEA[1,2] [*], Catalina CIMPEANU[1], Catalina BARNA[1], Marina ILIESCU[1]

[1] *Horia Hulubei National Institute of Physics and Nuclear Engineering, Măgurele, Romania*

[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Following the activities developed in a nuclear facility result gaseous and liquid radioactive effluents and radioactive solid waste. All these waste contain radioactive isotopes which are potentially pollutants for the environment.

According to the legislation, discharging of radioactive liquid and gaseous effluents into the environment, must meet the requirements of the unrestricted discharge (Norms on radioactive waste management (NDR) – issued by the National Commission for Nuclear Activities Control).

In this paper we present the case of liquid effluents discharged into the environment, containing the radioisotopes: 192Ir, 60Co, 241Am, 137Cs, 3H. Samples of the content of liquid effluents reservoirs were measured in order to determine the activity by gamma spectrometry for the gamma emitting radioisotopes (192Ir, 60Co, 241Am, 137Cs) and by liquid scintillation counting for tritium (3H).

The current legislation states annual derived emission limits for each radioisotope, the novelty of the present work consisting in the cumulative approach of these radioisotopes activity during 3.5 years of observation.

Keywords: superposition and cumulation of action radioactive pollutants, environment, radioisotopes, radioactive effluents

[*] Corresponding author: smanea@nipne.ro

APPLICATIONS OF CHEMICAL ENGINEERING PRINCIPLES AND THE LUMPING ANALYSIS IN MODELLING THE LIVING SYSTEMS – A TRADE-OFF BETWEEN SIMPLICITY AND MODEL QUALITY

Gheorghe MARIA[1*]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Living cells are organized, self-replicating, self-adjustable, evolvable and responsive structures to environmental stimuli. Due to the highly complex and partly unknown aspects of the metabolic processes, the detailed mathematical modelling at a molecular level remains still an unsettled issue, even if remarkable progresses and developments of extended simulation platforms have been reported. The general modelling rules, based on physico-chemical-biological & chemical engineering principles, and a statistical data treatment are more difficult to be applied to living systems. That is because metabolic cell processes present a low observability vs. the very large number of species (10^4), reactions (10^5), and transport parameters. Application of advanced lumping techniques can increase the model estimability by reducing the number of reactions and/or variables, and by keeping the most influential terms. Model quality tests, parameter and species sensitivity analysis, principal component and algorithms to find invariant subspaces are common rules to reduce extended model structures. The reduction cost is a loss of information on certain species and reactions, a loss in model generality, prediction capabilities, and physical meaning for some rate constants.

To overcome the structural low identifiability of living cell processes, the current trend is to use all types of information 'translated' from the 'language' of molecular biology to that of mechanistic chemistry, by preserving the cell structural hierarchy and species functions. Application of (bio) chemical engineering concepts and modelling methods, and of the nonlinear systems control theory allow improving the cell model quality, and may offer a detailed simulation of the cell metabolism adaptation to environmental changes, useful for designing modified genetic circuits and of modified micro-organisms.

Several case studies exemplify application of such a gradual lumping analysis and modular approach to derive valuable models able to mimic the stationary and perturbed cell growth, cell response to stimuli, and system homeostasis under isotonic osmolarity.

Applications refers to in-silico design of mutant cells with desirable motifs, such a genetic switches acting as biosensors, or genetic circuits amplifying exogeneous stimuli, or involved in signal transduction, or in oscillatory cell processes such as glycolysis. Another case study presents a multi-layer / multi-scale model that couples a structured representation of a metabolic genetic regulatory circuit at a molecular level with the macroscopic mass balances of the relevant state variables of a fluidized-bed bioreactor used for mercury uptake from wastewaters by using immobilized E. coli bacteria. The model was proved useful for process design and optimal control purposes allowing

---

[*] Corresponding author: gmaria99m@hotmail.com

predicting the wild/cloned bacteria metabolism adaptation (i.e. the response of the mer-operon expression) over several cell generations to dynamic operating conditions of the bioreactor.

In conclusion, general chemical engineering modelling principles are proved to be valuable tools for representing the both stationary and dynamic characteristics of the complex cell processes. Elaboration of reduced models of satisfactory quality is closely related to the ability of selecting the suitable lumping rules, key-parameters, and influential terms, and to apply multi-objective non-/conventional estimation criteria that realize the best trade-off between model simplicity and its predictive quality.

Keywords: kinetic modelling of cell metabolic processes; homeostatic regulation of gene expression; regulatory modules of gene expression (GERM); linking GERM-s

ELECTROSYNTHESIS AND ON-LINE MONITORING OF HYDROGEN PEROXIDE IN QUASI NEUTRAL MEDIA

Ana-Domnica M RINCEAN[1*], Sorin-Aurel DORNEANU[1,2], Petru ILEA[1,2]

[1] Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, 11 Arany Janos str., RO-400028, Cluj-Napoca, Romania

[2] Babes-Bolyai University, Interdisciplinary Research Institute on Bio-Nano-Sciences, 42 Treboniu Laurian str., RO-400271, Cluj-Napoca, Romania

Hydrogen peroxide (HP) is an environmentally friendly chemical that leaves non-hazardous residues, since it decomposes only to water and oxygen. Based on our previous results concerning the HP electrosynthesis (HPE) by the partial electro reduction of dissolved O_2 in strong alkaline media (1 M NaOH) [1, 2], we decided to implement the optimal operational parameters at a micro-pilot scale electrochemical reactor with recirculation and HP accumulation capability. In this context, we find that is mandatory to design and validate an accurate and reliable flow-through detector able to monitor, on-line and in-situ, the concentration of accumulated HP.

Many consecrated techniques for HP detection are inadequate for flow analysis, due to the requirement of permanent addition of specific reagents [3]. In order to overcome this problem, based on the ability of HP to present an intense absorption in the UV range, we decided to test the possibility to measure the HP concentration by spectrophotometry without addition of specific reagents.

The preliminary tests were successfully accomplished using diluted standard solution of HP ($1 \div 500$ ppm) prepared in bi-distilled water. Subsequently, when we try to repeat the same set of measurements in the presence of 0.1 M NaOH in the standard solutions, we observed an intense HP decomposition, for standard having concentrations equal or higher to/than 50 ppm. In these conditions and based on literature data [4], for all the further experiments, we decide to replace, the alkaline supporting electrolyte with a quasi neutral one, consisting in a 0.1 M Na_2SO_4 solutions. In these conditions, we conclude that de designed spectrophotometrical method for HP detection can be used successfully during the accumulation experiments, but only at concentration greater that 10 ppm. In order to decrease the detection limit under this value, an original dedicated 3-electrodes flow-through amperometric detector was designed and tested.

Finally, using the Pt/SG wall-jet ring-disc electrode system, the HPE process was studies in sulphate media, applying different electro-activation (EA) protocols. The experiments revealed that, the current efficiency of HPE process can increase from a value of 46 % (recorded for the unmodified graphite electrode) up to 52 % when the auto-adaptive galvanostatic multi-sequence EA protocol is used.

Keywords: hydrogen peroxide electrosynthesis, hydrogen peroxide detection, graphite electroactivation, wall-jet ring disk electrode, auto-adaptive techniques

---

* Corresponding author: ana_marincean@yahoo.com

References

[1] Vlaic C., Dorneanu S. A., Ilea P., *Studia Universitatis "Babe -Bolyai", Seria Chimia*, LIV(2), 167, 2011.

[2] Vlaic C., Dorneanu S. A., *Studia Universitatis "Babe -Bolyai", Seria Chimia*, LX(3), 141, 2015.

[3] Brandhuber P. J., Korshin G., *Methods for the Detection of Residual Concentrations of Hydrogen Peroxide in Advanced Oxidation Processes*, WateReuse Foundation, Alexandria, VA, chapter 2, 2009.

[4] Scialdone O., Galia A., Gattuso C., Sabatino S., Schiavo B., *Electrochimica Acta*, 182, 775, 2015.

DESIGN AND PLANTWIDE CONTROL OF A PROCESS FOR n-BUTYL ACRYLATE PRODUCTION

Mihai Daniel MORARU[1,2], Costin Sorin BÎLDEA[1*]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*
[2] *Dept. of Process Technology & Development, Hexion, The Netherlands*

n-Butyl acrylate is commercially produced from acrylic acid and n-butanol using strong acidic homogeneous catalysts. To overcome corrosion, catalyst removal from product and catalyst disposal problems after neutralization, research based on solid catalysis received increased attention in the recent years. However, design and control studies of an entire plant are rare. In this view, the design and control of two reactor-separator-recycle process alternatives are developed. Both use a fixed-bed reactor with Amberlyst 131. The separation of n-butyl acrylate from the mixture with n-butanol and acrylic acid is difficult. One of the process alternatives makes the separation by distillation at pressure above atmospheric, while the other conveniently employs extractive distillation with ethylene glycol. Both processes are controllable, the control system showing robustness when increase or decrease in production capacity is required, or operating conditions change. Aspen Plus and Aspen Plus Dynamics are used as efficient Computer-Aided Process Engineering tools.

Keywords: n-butyl acrylate, esterification, reactor-separation-recycle, bifurcation analysis, Aspen Plus.

---

* Corresponding author: s_bildea@upb.ro

LEAD REMOVAL FROM AQUEOUS SOLUTIONS BY CALCIUM ALGINATE AND CHITOSAN-CALCIUM ALGINATE – A COMPARATIVE STUDY

Noor Edin MOUSA[1*], Rodica-Elena P TESCU[1], Cristian ONOSE[1], Vasile LAVRIC[1], Claudia Maria SIMONESCU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

The removal of lead (II) from aqueous solutions through adsorption onto biopolymer sorbents, such as calcium alginate (CA) and chitosan coated calcium alginate (CCCA), was studied using equilibrium batch technique.

The two adsorbent materials were prepared by a simple synthesis method. Calcium alginate was obtained from sodium alginate and $CaCl_2$ solution. Coating calcium alginate with chitosan enhanced sorption and mechanical properties of this new material [1].

CA and CCCA were characterized using infrared spectroscopy (FT-IR) to highlight the main functional groups that could be involved in lead bonding, and also to elucidate the mechanism involved in the reaction between alginate and chitosan.

CA and CCCA were tested for lead removal from synthetic aqueous solutions. The quantity of lead ions adsorbed depends on the initial pH solution, lead concentration and temperature. The adsorption capacity and the removal efficiency are higher for CCCA than CA. These results are in accordance with other published data [1-4]. The thermodynamic studies proved that the adsorption of lead ions onto both CA and CCCA materials is an endothermic spontaneous process, thus increasing the temperature improves adsorption performances [5].

The adsorption capacity of lead onto CA and CCCA is well fitted by Freundlich adsorption isotherm. This may suggest that lead adsorption onto CA and CCCA is governed by a multilayer process on a heterogeneous surface [6].

The adsorption rate is well modeled by a pseudo-second-order kinetic, with the chemical sorption as the rate-limiting step [7, 8].

The adsorption capacity and removal efficiency recommend CCCA as better removal material for lead ions, although CA has its merits. Further energetic and economic studies are needed to choose between them.

Keywords: chitosan/ alginate, lead removal

---

* Corresponding author: adin_noor@yahoo.com

References

[1] Vijaya Y., Popuri S.R., Boddu V.M., Krishnaiah A., Modified chitosan and calcium alginate biopolymer sorbents for removal of nickel (II) through adsorption, *Carbohydr. Polym.*, 72, 261-271, 2008.

[2] Rashid M., Khan F., Lutfullah, Removal of Pb(II) ions from aqueous solutions using hybrid organic–inorganic composite material: Zr(IV) iodosulphosalicylate, *J. Water Proc. Eng.*, 3, 53-61, 2014.

[3] Wu F.-C., Tseng R.-L., Juang R.-S., A review and experimental verification of using chitosan and its derivatives as adsorbents for selected heavy metals, *J. Env. Manag.*, 91, 798-806, 2010.

[4] Zhou L.M., Wang Y.P., Liu Z.R., Huang Q.W., Characteristics of equilibrium, kinetics studies for adsorption of Hg(II), Cu(II), and Ni(II) ions by thiourea-modified magnetic chitosan microspheres, *J. Hazard. Mater.*, 161, 995-1002, 2009.

[5] Tran H.N., You S.-J., Chao C.-P., Thermodynamic parameters of cadmium adsorption onto orange peel calculated from various methods: A comparison study, *J. Env. Chem. Eng.*, 4(3), 2671-2682, 2016.

[6] Ibrahim M.B., Sani S., Comparative Isotherms Studies on Adsorptive Removal of Congo Red from Wastewater by Watermelon Rinds and Neem-Tree Leaves, *Open Journal of Physical Chemistry*, 4, 139-146, 2014.

[7] Ho Y.-S., McKay G., A comparison of chemisorption kinetic models applied to pollutant removal on various sorbents, *Trans. Inst. Chem. Eng.*, 76B, 332-340, 1998.

[8] Chen X., Modeling of Experimental Adsorption Isotherm Data, *Information*, 6, 14-22, 2015.

AMMONIA ADSORPTION KINETCS ON THE CLAY PARTICLES IN FLUIDIZED BED

Gabriela MUNTIANU[1*], Ana Maria GEORGESCU[1], Ileana Denisa NISTOR[1], Gheorghi a JINESCU[2], Gholamreza DJELVEH[3]

[1]*"Vasile Alecsandri" University of Bac u, Faculty of Engineering, Department of Chemical and Food Engineering, 157 Calea M r e ti Street, 600115 Bacau, Romania*

[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[3] *Clermont Université, ENSCCF, Pascal Institute, GePEB axis, UMR CNRS 6602, 24 avenue des Landais, BP 2016, Aubière, Clermont Ferrand, France*

The fluidized bed was used to intensify the adsorption process of ammonia on commercial clay particles. Clay particles of different densities and specific surface area were used as adsorbent bed for ammonia molecules. The fluidized bed is formed when the gas velocity of the mixed gases (air and ammonia) circulating through the adsorbent bed, is equal with the minimum fluidization velocity ($U_g=U_{mf}$). To intensify the adsorption process the fluidized bed was used for improving the gas-particles contact. Mixing the clay particles leads to a higher surface contact with the ammonia.

The behavior of commercial clay particles were studied in the fluidized bed in different conditions. The aim of this paper is the use of a suitable adsorbent that could be available in nature, cheap and that can be easy to regenerate. The commercial clays were characterized by three analyses: the mineralogical composition by X-ray diffraction, the particle size by laser diffraction and the thermal behavior by thermo gravimetric analysis.

The experimental researchers conclude that the commercial clays are good adsorbents for the adsorption of ammonia. The adsorption capacity was determined in different conditions. The best results were obtained when using the fluidized bed with particle beds heights over 10 cm.

Keywords: ammonia, adsorption capacity, commercial clays, fluidized bed

* Corresponding author: muntianu.gabriela@yahoo.com

STUDIES REGARDING SUCCINIC ACID SYNTHESIS

Cristina ORBECI[1*], Daniela Simina TEFAN[1, 2], Mircea TEFAN[3], Rodica ANGHEL[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[2] *IPROCHIM S.A. 19-21 M. Eminescu Street, Bucharest 1, Romania*

[3] *University Titu Maiorescu, Pharmacy Faculty, Dâmbovnicului 22 Street, 040441, Bucharest-4, Romania1*

Biotechnologies are increasingly used at industrial level and replace chemical synthesis technologies. Transforming natural raw materials is mediated by microorganisms or enzymatic mixtures.

Getting succinic acid ($C_4H_6O_4$) has special significance for the market foodstuffs and pharmaceuticals, surfactants, detergents, solvents green food ingredients, feed additives and biodegradable plastics but also for the synthesis of: polyurethanes, resins, polybutylene, succinate and plasticizers. In the food industry succinic acid is used as additive (E 363), flavor enhancer and acidity regulator. It is found in soups, soft drinks and sweets [1].

Succinic acid can be produced in hydrogenation processes of maleic acid, fumaric acid or maleic anhydride with standard catalysts such as Raney-nickel, Cu, Pd-Al_2O_3, Pd-$CaCO_3$. Also it is obtained by fermentation of glucose. The raw materials used for producing succinic acid are wheat, corn, glucose or sucrose [2, 3].

Today the researchers aim at obtaining biotechnologies more efficiently than the ones based on petroleum products [2 - 5].

The goal of present work is obtaining of succinic acid from maize. In the first stage it used a mixture of enzymes Termamyl SC and San Extra L for obtaining fermentable glucose in cornstarch. Fermentable glucose has undergone fermentation process in the presence of *Saccharomyces Cerevisiae* to obtain alcohol and succinic acid.

In order to emphasize the degree of conversion of starch from maize as well as the conversion of the fermentable sugar to alcohol it was measured glucose concentration using refractive index and concentration of dry concentration.

Highlighting composition for the final fermentation mixtures they were performed FTIR spectral analysis, and chromatographic analysis. Even if the concentration of succinic acid obtained has not reached remarkable values was founded an experimental model that will improve.

Keywords: biotechnologies, fermentation, succinic acid, starch from maize, fermentable sugar, glucose.

References

[1] Song H., Lee S.Y., *Production of succinic acid by bacterial fermentation*, Enzyme and Microbial Technology, 39 (3), 352–361, 2006.

Corresponding author: cristina.orbeci@upb.ro

[2] Rubin E.M., *Catalytic processes and catalyst development in biorefining, Genomics of cellulosic biofuels,* Nature, 454, 841 – 845, 2008.

[3] Alonso M.D., Bond J.Q., Dumesic J.A., *Catalytic conversion of biomass to biofuels*, Green Chemistry, 12, 1493 – 1513, 2010.

[4] Rena H., Girisutac B., Zhoua Y., Liu L., *Selective and recyclable depolymerization of cellulose to levulinic acid catalyzed by acidic ionic liquid*, Carbohydrate Polymers, 117, 569–576, 2015.

[5] Choudhary H., Nishimura S., Ebitani K., *Metal-free oxidative synthesis of succinic acid from biomass-derived furan compounds using a solid acid catalyst with hydrogen peroxide*, Applied Catalysis A: General, 458, 55– 62, 2013.

INCREASING THE DEGREE OF TREATMENT FOR CCOCr AND CBO5 USING AQUA PE TYPE MICROORGANISMS IN COMBINATION WITH ACTIVATED SLUDGE

Ca en PANAITESCU[1*]

[1] *Petroleum-Gas University of Ploiesti, Blvd. Bucure ti, no. 39, Ploie ti, 100680, Romania*

Industrial wastewater treatment is necessary for two main reasons: to limit the amount of wastewater discharged uncontrolled in the receiver's water and to reduce the impact on the environment, reuse of treated water. In this study, industrial wastewater with a COD (Chemical Oxygen Demand) content over 600 mg/L and CBO5 over 300 mg/L was monitored, and increasing the degree of treatment by mixing activated sludge with selected microorganisms was considered. For this Aqua Micropan PE type microorganiosms were used. AQUA PE type microorganisms protect the environment, widely reduce ammonia dissolved in water, COD phosphates and BOD5. In this way we were interested in increasing the degree of purification of the biological level by increasing the activity (dynamics) of microorganisms. The activity of the biomass formed in the laboratory was observed for 12 weeks. After the addition of microorganisms, aeration was achieved throughout experiments until dissolved oxygen concentration reached a value of 4 ppm. After the study's completion we noticed a decline in CBO5 and CCO values as follows: COD dropped from 520 mg/L to 115 mg/L; CBO5 dropped from 320 mg/L to 18 mg/L. The decrease of these values means a correct treatment and an increase in the degree of purification. To estimate the change over time in the number of individuals composing the population studied we turned to determined the dynamics of the population of microorganisms. Following the experiment conducted in the laboratory, we demonstrated that treatment with PE Aqua Micropan microorganisms can be effective and can increase the degree of treatment in combination with activated sludge/mud. It can be successfully applied in treatment plants of industrial wastewater.

Keywords: CCOCr, CBO5, PE Aqua Micropan microorganisms.

References
[1] Panaitescu C., Onutu I., Monitoring the quality of the sludge resulted from domestic wastewater treatment plants and the identification of risk factors, *Environmental Engineering and Management Journal*, vol. 12, no. 2, 351-358, 2013.
[2] Panaitescu C., Bucuroiu R., Study on the composition of municipal waste in urban areas of prahova county, *Environmental Engineering and Management Journal*, Vol. 13, No. 7, 1567-1571, July 2014.

* Corresponding author: cpanaitescu@upg-ploiesti.ro

THE IMPLEMENTATION OF THE COAGULATION– FLOCCULATION PROCESS IN THE LEACHATE TREATMENT FROM ECOLOGICAL LANDFILLS

Caŧen PANAITESCU[1*], Gabriela STAN[1]

[1] *Petroleum-Gas University of Ploiesti, Blvd. Bucureŧti, no. 39, Ploieŧti, 100680, Romania*

The application of the coagulation-flocculation process in the treatment of leachate is not a normal process, because its load with pollutants is very high and the solution is not uniformly ionized. Coagulation-flocculation applies especially to surface waters or wastewaters (when their recirculation is desired) and does not apply to groundwaters, which have a very low content of colloids.

Variants were tested in the current study in which polyelectrolyte type coagulants and flocculants were mixed, so that removing material type suspended pollutants and organic matter was made by agglomeration of colloids in floaters - larger and heavier units. Turbidity occured and it was reduced through the process of coagulation - flocculation. The experimental study conducted was based on the concept of operational research, namely:

- − Stating the issue (Problem Formulation);
- − The stability of the mathematical model system studied;
- − Obtaining the optimal solution;
- − Testing of the model, solution and influence parameters;
- − Applying the solution's results in experimental studies.

The discovered solution treatment was applied in leachate treatment plants, the results being presented in the current study. It has been demonstrated that the transition from the laboratory scale to the industrial scale was successful, and the environmental impact has been significantly reduced through the advanced treatment of the leachate.

Keywords: coagulation, flocculation, leachate, parameters.

References
[1] Stratula C., Panaitescu C., Lungu A., Some considerations concerning the advanced elimination on epychlorhydrin from 1,2-dichloropropane by fractioning, *Revista de chimie*, vol. 56, no.6, 677-681, 2005.

───────────────

[*] Corresponding author: cpanaitescu@upg-ploiesti.ro

THERMODYNAMIC INVESTIGATION OF SOME MIXED MONOLAYERS AT THE AIR WATER INTERFACE

Roxana-Diana PAȘCA[1*], Ossi HOROVITZ[1]

[1] *"Babes-Bolyai" University of Cluj-Napoca, Faculty of Chemistry and Chemical Engineering, Chemical Engineering Department, Kogalniceanu Str., no. 1, 400028, Cluj-Napoca, Romania*

The principal thermodynamic function used to characterize the behavior of a mixed monolayer at the air-water interface is the surface excess Gibbs energy (ΔG_{ex}), calculated for different mole fractions. A minimum of the function shows a high stability of the monolayer studied. The surface excess Gibbs energy was calculated for many biochemical systems, such as: sulfatide/ dipalmitoylphosphatidylcholine (DPPC), sulfatide/ 1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine (DPPE) [1], sulfatide/ cholesterol [2], monogalactosyldiacylglycerol/ubiquinone [3], DPPC/ tetramyristoyl cardiolipin (TMCL) [4], cholesterol/DPPC mixed monolayers on water with prazosin [5], edelfosine and cholesterol [6], DPPC/ dioctadecyldimethylammonium bromide (DODAB), DODAB and oleic acid (OA), DPPC/OA [7], DPPC/ bacteriochlorophyll c [8], DPPC with 3-monopalmitoyl glycerol (PG) and DPPC with palmitic acid 4-methylumbelliferyl ester (4-MU) [9], dioleoyltrimethylammonium propane (DoTAP)– DPPC and DoTAP –dipalmitoyphosphatidylglycerol (DPPG) [10], 1-stearoyl-2-oleoyl-sn-glycero-3-phosphocholine (PC) and 1-stearoyl-2-oleoyl-sn-glycero-3-phospho-l-serine sodium salt (PS) [11].
A comparison of the values obtained and their significance is presented in this study.

Keywords: surface excess Gibbs energy, lipids.

References
[1] Sun R., Hao C., Zhang J., Chang Y., Niu C., A monolayer study on phase behavior and morphology of binary mixtures of sulfatides with DPPC and DPPE, *Colloids and Surfaces B: Biointerfaces*, 73(2), 161–167, 2009.
[2] Hao C., Sun R., Zhang J., Chang Y., Niu C., Behavior of sulfatide/cholesterol mixed monolayers at the air/water interface, *Colloids and Surfaces B: Biointerfaces*, 69(2), 201–206, 2009.
[3] Hoyo J., Torrent-Burgues J., Guaus E., Biomimetic monolayer films of monogalactosyldiacylglycerol incorporating ubiquinone, *Journal of Colloid and Interface Science*, 384(1), 189–197, 2012.
[4] Etienne F., Roche Y., Peretti P., Bernard S., Cardiolipin packing ability studied by grazing incidence X-ray diffraction, *Chemistry and Physics of Lipids*, 152(1), 13–23, 2008.
[5] Gzyl-Malcher B., Handzlik J., Klekowska E., Interaction of prazosin with model membranes — A Langmuir monolayer study, *Bioelectrochemistry*, 87, 96–103, 2012.
[6] Wiȩcek A., Dynarowicz-Łątka P., Miñones J. Jr., Conde O., Casas M., Interactions between an anticancer drug – edelfosine – and cholesterol in Langmuir monolayers, *Thin Solid Films*, 516(24), 8829–8833, 2008.

---

* Corresponding author: roxana_diana_pasca@yahoo.com, roxana.pasca@ubbcluj.ro

[7] Goncalves da Silva A. M., Romao R. I. S., Mixed monolayers involving DPPC, DODAB and oleic acid and their interaction with nicotinic acid at the air–water interface, *Chemistry and Physics of Lipids*, 137(1-2), 62–76, 2005.

[8] Dudkowiak A., Biadasz A., Bartczak A., Spectral and thermodynamic characterization of bacteriochlorophyll c and dipalmitoylphosphatidylcholine in the binary mixed monolayers, *Journal of Molecular Structure*, 887(1-3), 128–134, 2008.

[9] Gzyl-Malcher B., Paluch M., Studies of lipid interactions in mixed Langmuir monolayers, *Thin Solid Films*, 516(24), 8865–8872, 2008.

[10] Panda A. K., Vasilev K., Orgeig S., Prestidge C. A., Thermodynamic and structural studies of mixed monolayers: Mutual mixing of DPPC and DPPG with DoTAP at the air–water interface, *Materials Science and Engineering C*, 30(4), 542–548, 2010.

[11] Luna C., Stroka K. M., Bermudez H., Aranda-Espinoza H., Thermodynamics of monolayers formed by mixtures of phosphatidylcholine/phosphatidylserine, *Colloids and Surfaces B: Biointerfaces*, 85(2), 293–300, 2011.

TRENDS INTO OF THE PROPYLENE – PROPENE DISTILLATION SIMULATION USING UNISIM DESIGN SIMULATOR

Cristian PĂTRĂŞCIOIU[1*], Minh Ahn CAO[1]

[1] *Petroleum-Gas University of Ploiesti, Blvd. Bucureşti, no. 39, Ploieşti, 100680, Romania*

The propylene – propene distillation process is an important source to make the poly-propylene and the plastics. The distillation process is known but in same time the process is very complex. The distributed and the multivariable character represent two important characteristics of this process [1]. Many studies refer to classically industrial distillation process that contains a distillation column, a condenser and a reboyler. A special case is the simulation of the distillation process with the thermal pump.

The classically distillation process simulation may be realized using the Unisim Design simulator [2]. The graphically object library of the simulator contains the *Distillation Column* module, that represents a mathematical model of the classically distillation column. The simulator configuration has been realized for a propylene – propene distillation process, the process objective being the quality specifications for distillated product, $x_D^i = 99.6\%$, respectively $x_B^i = 4.14\%$ for the bottom product. The numerical simulations have been realized for a domain of the feed flow rate. The simulation results have been used to present the temperature distribution, internal flows rate distribution, molar mass and liquid density. Also, the data base results will be used to compare the classical distillation process simulations with the simulation results of the distillation process with the thermal pump.

The distillation columns with the thermal pump are structural different with the classical distillation process. So, the condenser existing in classical structure is eliminated and the vapors from the top column are compressed and ulterior they are used than thermal flow into column reboyler [3]. The vapors are condensed using detent valve and ulterior they are collected in reflux vessel. From reflux vessel they is extracted the reflux flow and the distillated product. The bottom column remains unchanged refer classical distillation column.

The authors have studied the possibility of the simulation of the distillation column with thermal pump. The simulation diagram design expects three steps: the emulation of the distillation column using the mathematical absorption model; the setting of the absorption model specifications to the distillation column requirements; the simulation diagram completion with thermal pump equipment [4].

The distillation column emulation using the absorption model is possible if the *Reboiled Absorber* module is used. The *Reboiled Absorber* module must to be configured with reboyler. A special attention was been accorded to implement the *Recycle* function. This function assures the concordance between the composition of the reflux flow (imposed by user) and the calculated composition of the outlet flow of the reflux vessel. The

---

[*] Corresponding author: cpatrascioiu@upg-ploiesti.ro

simulation diagram has been tested in same conditions as well as tests with the classical distillation column. Because there has been obtained the approached results, the substitute of the *Distillation Column* model with model is possible.

The differences between the results obtained by those mathematical models are generated by the different specification of the reflux composition. The authors have been developed a special technique offered by *Unisim Design*. So, there has used two mathematical models, respectively *Distillation Column* and *Reboiler Absorption* in same simulation diagram. The *Distillation Column* module generates the reflux composition. A special function permits the export of the concentration values of the reflux flow form the *Distillation Column* module into *Reboiler Absorption* module. The new simulations have validated the proposed simulation diagram.

Keywords: distillation, absorption, simulation, Unisim Design

References

[1] Patrascioiu C., Cao Minh Anh, Popescu M., Control of propylene - propane distillation process using Unisim Design, *19th International Conference on System Theory, Control and Computing*, October 14 - 16, 2015, Cheile Gradistei - Fundata Resort, Romania, p. 747 – 752.

[2] Patrascioiu C., Paraschiv N., Anh Cao Minh, Popescu M., Robust Control of Industrial Propylene-Propane Fractionation Process, *Computer Aided Chemical Engineering*, 37, 1745-1750, 2015.

[3] Donald F. Sneider, *Heat Integration Complicates Heat Pump Troubleshooting*, Stratus Engineering, Don Sneider, 2001.

[4] Patrascioiu C., Modelling and Simulation of the Freezing Systems and Heat Pumps Using Unisim® Design, *International Journal of Chemical, Molecular, Nuclear, Materials and Metallurgical Engineering*, Vol:10, No:5, 514-519, 2016.

CHLORINE DIOXIDE – ALTERNATIVE OXIDANT IN THE TREATMENT OF DRINKING WATER SUPPLIES

Cristiana COSMA[1], Viorel P TROESCU[1*], Olga TIRON[1], Valeriu B DESCU[1], Alina-Monica MARE [2], Gheorghi a JINESCU[2]

[1] *National Research and Development Institute for Industrial Ecology – INCD ECOIND, 71-73 Drumul Podu Dambovitei Street, Sector 6, 060652, Bucharest, Romania*
[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Chlorine dioxide (ClO_2) is a highly reactive oxidant and disinfectant agent. A common application of ClO_2 in drinking water has been for control of tastes and odours associated with algae from surface water or for conversion of oxidizable Mn(II) + Fe(II) in precipitable species, especially for groundwater containing also low concentrations of ammonium ions.
A case study for the pretreatment of a surface water source with different microalgae species (chlorophyll "a" = 2.4 µg/L) and soluble organic matter (DOC = 5.6 mgC/L) using ClO_2 solution is presented.

Key words: chlorine dioxide, surface water, microalgae species, DOC, degradation/ oxidation

---

* Corresponding author: patroescuv@yahoo.com

PREPARATION AND CHARACTERIZATION (ENTRAPMENT EFFICIENCY) OF TRANSFEROSOMES WITH *SAMBUCUS EBULUS* LEAVES EXTRACT

Ramona-Daniela PĂVĂLOIU[1*], Corina BUBUEANU[1], Sha'at FAWZIA[1], Daniela-Crina SĂLCEANU[1], Adriana VOICULEȚ[1], Cristina HLEVCA[1]

[1] *National Institute for Chemical-Pharmaceutical Research and Development - ICCF Bucharest, Vitan Avenue 112, 3rd District, Bucharest, Romania.*

Extensive research is directed on incorporation of plant extract or herbal drugs in innovative drug delivery systems, like lipid vesicles (liposome, transfersome, phytosome, ethosome, etc). Application of these innovative techniques could minimize certain limitations of plant extract such as: poor solubility, toxicity, degradation in gastrointestinal media [1, 2]. The aim of the paper was to study the entrapment of Sambucus ebulus leaves extract in transferosomes with the purpose to obtain an innovative drug delivery system for this compound. Sambucus ebulus L. (dwarf elder, fam. Adoxaceae) is a perennial plant widespread in Europe with antioxidant, anti-inflammatory, antinociceptive, antimicrobial, antiarthritic, anticancer properties [3, 4].

The Sambucus ebulus leaves raw material was harvested in august 2015 from the south of Romania and extracts were obtained by extraction with ethanol 50% (v/v). The plant extract was characterized using high performance thin layer chromatography (HPTLC) for the determination of qualitative phytochemical content, and the Folin-Ciocalteu method for the determination of quantitative evaluation of total polyphenolic content. Transferosomes with Sambucus ebulus extract were prepared by film hydration method followed by sonication; several parameters were varied: the amount of phosphatidylcholine and sodium cholate, the amount of plant extract, the time of sonication. The entrapment efficiencies of transferosomes with Sambucus ebulus extracts were evaluated.

The phytochemical screening of Sambucus ebulus leaves extract revealed the presence of flavonoid glycosides, rutin, hyperoside, and chlorogenic acid and high total phenol content. The evaluation of transferosomes with Sambucus ebulus leaves extract showed good entrapment efficiency. The results suggest that transferosomes could be exploited as carriers for plant extracts in biomedical or in cosmetic applications, although further investigations are needed.

Keywords: transfersome, plant extract, Sambucus ebulus

References
[1] Bhattacharya S., Phytosomes: Emerging Strategy in Delivery of Herbal Drugs and Nutraceuticals, *Pharma. Times*, 41 (3): 9-12, 2009
[2] Pawar H. A., Bhangale B. D., Phytosome as a Novel Biomedicine: A Microencapsulated Drug Delivery, System, *J. Bioanal. Biomed,* 7 (1): 006-012, 2015.

---

* Corresponding author: pavaloiu_daniella@yahoo.com

[3] Tasinov O., Kiselova-Kaneva Y., Ivanova D., Sambucus ebulus - from traditional medicine to recent studies, *Scripta Scientifica Medica*, 45 (2): 36-42, 2013.

[4] Rodino S., Butu A., Petrache P., Butu M., Dinu-Pirvu C. E., Cornea C. P., Evaluation of the antimicrobial and antioxidant activity of *Sambucus Ebulus* extract, *Farrnacia*, 63 (5): 751-754, 2015.

OPTIMIZATION OF VOLATILE ORGANIC COMPOUNDS REMOVAL BY PACKED-BED ABSORPTION

Mihai CERNAT[1], Oana Cristina PÂRVULESCU[1;], Tănase DOBRE[1], Ioana MAIOR[2]

[1]Department of Chemical and Biochemical Engineering, University POLITEHNICA of Bucharest, 1-7 Polizu Street, 011061, Bucharest, Romania

[2]Department of Inorganic Chemistry, Physical Chemistry and Electrochemistry, University POLITEHNICA of Bucharest, 1-7 Polizu Street, 011061, Bucharest, Romania

Volatile organic compounds (VOCs) can be removed from gas streams using destructive (*e.g.*, thermal and catalytic oxidation, bio-filtration) or recuperative (*e.g.*, adsorption, absorption, condensation, membrane separation) abatement techniques. Gas-liquid absorption in counter-current packed-bed columns is a simple and effective regenerative technique which is widely used to transfer VOCs from a gas phase into a liquid absorbent [1]. To avoid uneconomic intensive operation, the total annual cost in terms of payback and operating costs should be estimated. Payback costs commonly refer to those of column and packing, whereas operating costs consider the power necessary to pump the gas and liquid phases [2]. The total cost depends on various parameters including gas flow rate, VOC type and initial concentration, absorbent type, column material and dimensions, packing type, material and dimensions, absorption efficiency, annual depreciation rate, process temperature and pressure.

A theoretical study on the modelling of acetone absorption from an air stream into water using a counter-current packed-bed column was presented. The influence of air mass flux (0.7-2.2 kg/(m^2·s)) on the total annual cost was studied under the following conditions: 1.2 m^3/s inlet volumetric gas flow rate, 0.03 inlet acetone mole fraction in the gas phase, clean absorbent, stainless column, 25×25×3 mm metallic Raschig rings, 95% separation efficiency, 10% annual depreciation rate, 21°C and 1 atm. An algorithm for determining the optimum gas mass flux leading to a minimum total annual cost was described. Pressure drop over the unwetted and wetted column, partial mass transfer coefficients, packing height and pumping gas cost increased as well as packing volume and payback cost decreased with an increase in gas mass flux. The lowest total annual costs, *i.e.*, 4745-4759 EUR/year, were achieved for gas mass fluxes in the range of 1.20-1.56 kg/(m^2·s), corresponding to gas superficial velocities of 1-1.3 m/s.

Keywords: Absorption, Modelling, Packed-bed column, Volatile organic compound

References

[1] Dumont E., Darracq G., Couvert A., Couriol C., Amrane A., Thomas D., Andrès Y., Le Cloirec P., Hydrophobic VOC absorption in two-phase partitioning bioreactors; influence of silicone oil volume fraction on absorber diameter, *Chemical Engineering Science*, 71, 146–152, 2012.

[2] Brunazzi E., Nardini G., Paglianti A., An economical criterion for packed absorption column design, *Chemical and Biochemical Engineering Quarterly*, 15, 199–206, 2002.

---

[*] Corresponding author: oana.parvulescu@yahoo.com

STUDIES ON THE GERMINATION CHANGE OF PLANTS AFTER DECONTAMINATION OF SOILS THAT ARE POLLUTED WITH CRUDE OIL

Maria POPA[1*]

[1] *Petroleum-Gas University of Ploiesti, Blvd. Bucure ti, no. 39, Ploie ti, 100680, Romania*

This paper is part of a comprehensive study on soil pollution with liquid petroleum products. It is known that soil affect plants through its physical characteristics, chemical (nutrients content, pH) and biological.

In developed countries, as well as in Romania produced numerous technical incidents that lead to changes in soil quality. An enumeration of the types of incidents may include: discharge of crude oil, salt water and drilling fluids in oil exploitation in the area of extraction and probes scaffold-extraction, drilling, contamination of the soil, subsoil and groundwater in the area of transport pipe of crude oil and fuels due to breakage of pipes for various reasons, traffic accidents and the railway involving specific means of transport (tanker), technical incidents in technological installations and tanks of oil refineries and petrochemical enterprises.

The coordinator of an action of a compliant ground contaminated with petroleum products must bear in mind when choosing and implementing a remediation technologies four determinants: the final remediation degree desired or required, duration of the remediation actions, the total cost required to conduct routine cleaning, side effects produced during the implementation of pollution control technologies and their application.

Remediation technologies of soil contaminated with petroleum products do not respond optimally while the four factors listed.

Soil is key to environmental pollutants tanks, storage and persistence of pollutants in soil are dependent on a number of factors: the exchange of air, the burying of pollutants and their biodegradability.

This paper aims to emphasize the germination of plants after a polluted soil sample was decontaminated by an extraction method, successive extraction with solvents. The soil sample was polluted with 5% crude oil. The soil sample was characterized by capillarity, establishing maximum height for water and for crude oil, permeability for water and for crude oil and granulometry. Knowing the average permeability can be determined and the corresponding retention capacity for water and for crude oil. Restoration potential for germination and soil analyzed to determine the presence of nutrients required before and after remediation. Were analyzed nutrients nitrogen, phosphorus and potassium.

---

[*] Corresponding author: mariapopa2007@gmail.com

References

[1] Patrascu C., Negoita L., Popa M., *Depoluarea solurilor contaminate cu produse petroliere, Lucrări de laborator*, Editura UPG – Ploieşti, ISBN 978-973-719-243-1, 2008.

[2] Boros M. N., Micle V., *Study on the application of phytoremediation of contaminated industrial sites*, Land Reclamation, Earth Observation Surveying, Environmental Engineering, Volume III, Bucharest, ISSN 2285-6064, ISSN-L 2285-6064, 99-106, 2014.

[3] Pavel L. V., Gavrilescu M., Overview of ExSitu Decontamination Techniques for Soil Cleanup, *Environmental Engineering and Management Journal*, Nov-Dec, vol.7, No.6, 815-834, 2008.

[4] Popa M., Negoiţă L., Rădulescu S., Techniques for Remediation of Soils Contaminated with Liquid Petroleum Products for Ecological, *Buletinul UPG, Seria Tehnica*, Vol. LXII, No.3A, ISSN 1224-8495, 70, 2010.

[5] Popa M., *Comparative studies on remediation techniques in laboratory of soils contaminated with oil products*, Land Reclamation, Earth Observation & Surveying, Environmental Engineering, Volume III, Bucharest, ISSN 2285-6064, ISSN-L 2285-6064, 13-16, 2014.

[6] Popa M., *Laboratory studies on the simulation of accidental pollution of soils, Land Reclamation*, Earth Observation & Surveying, Environmental Engineering, Volume IV, Bucharest, ISSN 2285-6064, ISSN-L 2285-6064, 116-119, 2015.

[7] Shirdam R., Zand A. D., Bidhendi G. N., Mehrdadi N., Phytoremediation of hydrocarbon contaminated soils with emphasis on the effect of petroleum hydrocarbons on the growth of plant species, *Phytoprotection*, vol.89, nr.1, 21-29, 2008.

[8] Yi Y. M., Park S., Munster C., Kim G., Sung K., Changes in Ecological Properties of Petroleum Oil-Contaminated Soil After Low-Temperature. *Thermal Desorption Treatment, Water, Air & Soil Pollution*, 227:108, Springer Journals, April 2016.

STUDY OF CERTAIN BENEFICIAL MINERAL CONTENT IN VARIOUS PLANT ORGANS

Mariana POPESCU[1*], Viorica TAMA [1], Andreea COZEA[1], Natalița BORDEI[1]

[1]*S.C. HOFIGAL EXPORT-IMPORT S.A., Intr. Serelor street, no.2, district 4, Bucharest, Romania*

The study aims to characterize the comparative content of beneficial minerals (iron, calcium, magnesium, manganese) in various organs of plants (root, stem, leaves, flowers) present in plant materials native: marigold (Calendula officinalis), french marigold (Tagetes patula), nettle (Urtica dioica), echinacea (Echinacea angustifolia), using the atomic absorption spectrometry (AAS) technique.

The experimental study showed different distribution of the minerals studied, preferential, depending on the plant organs.

Plants studied, from organic sources will be used as raw materials for making food supplements with effect in the prevention of certain diseases.

Keywords: flame atomic spectrometry, heavy metals, plant organs, marigold, french marigold, nettle, echinacea.

References

[1] Luis A. Valdez-Aguilar, Catherine M. Grieve, James Poss, Donald A. Layfield, *Salinity and Alkaline pH in Irrigation Water Affect Marigold Plants: II. Mineral Ion Relations*, Hort Science, vol. 44(6), p.1726–1735, 2009.

[2] Cozea A., Ionescu (Bordei) N., Popescu M., Neagu M., Gruia R., *Comparative study of the composition of some oil cakes with phytotherapeutical potential*, Rev. Chim. (Bucharest), 67 (3), p. 422-425, 2016.

[3] Joanne Barnes et col., *Herbal medicines*, 3rd Ed., Published by the Pharmaceutical Press, Londra, UK, 2007.

[4] Indrayan A.K., Sharma S., Durgapal D., Kumar N., *Determination of nutritive value and analysis of mineral elements for some medicinally valued plants from Uttaranchal*, Curent Science, vol. 89, pp. 1252-1255, 2005.

[5] Bertoni J., col. *Biological Inorganic chemistry-Structure and reactivity*, University Science Books, Sansalito-California, 2007.

---

* Corresponding author: mari.popescu@yahoo.com

DOXORUBICIN FUNCTIONALIZED MAGNETITE NANOPARTICLES- ENHANCERS IN RADIOTHERAPY

Roxana-Cristina POPESCU[1,2*], Ecaterina ANDRONESCU[2], Andrei I. APOSTOL[1], Cosmin MUST CIOSU[1], Roxana TRU C [2], Bogdan VASILE[2], George Dan MOGO ANU[3], Laurenţiu MOGOAN [3], Alexandru Mihai GRUMEZESCU[2], Diana SAVU[1]

[1]*„Horia Hulubei" National Institute for Physics and Nuclear Engineering, Magurele, Romania;*

[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[3]*University of Medicine and Pharmacy of Craiova, Romania;*

Nanotechnology has been currently used in the fabrication of targeted carriers for anti-tumor substances, as one solution for exceeding the tumor cells resistance to classical treatment schemes. Even if there are several Food and Drug Administration- approved nano-systems, there is still a continuous urge to find more effective treatment options, which are supposed to overcome the shortcomings of the existing ones. We propose the obtaining of different drug delivery systems based on magnetite nanoparticles cores and doxorubicin chemotherapeutic substance, in order to obtain specific toxic responses in human cancer cells. These were fabricated using a Massart- modified co-precipitation method.

The nanoparticles characterizing was done in terms of crystallinity, chemical composition and structure: X-Ray diffraction (XRD) and Selected Area Electron Diffraction (SAED) helped identify the samples, their high level of crystallinity being proven through the same methods and confirmed through High resolution Transmission Electron Microscopy (HRTEM); the functionalization of magnetite with anti-tumor substances was highlighted through the thermogravimetric analysis (TGA) and the hydrodynamic analysis through Dynamic Light Scattering (DLS).

Regarding the biological effects, the *in vitro* cytotoxic potential was proved for an osteosarcoma tumor model (based on MG-63 cell line), using both quantitative (MTT tetrazolium-salt viability assay, Lactate Dehydrogenase Assay, Reactive Oxygen Species measurement, Micronuclei assay, Comet Assay) and qualitative estimations (F-actin immunofluorescence staining, fluorescence microscopy cellular entrapment evaluation, scanning electron microscopy), correlated with the quantitative determination of nanoparticles cellular entrapment efficiency using particle induced X-ray emission technique (PIXE).

These nanaoparticles determine the apparition of reactive oxygen species, which eventually lead to genotoxic effects in cancer cells. The tumor cell death is accelerated by applying low dose ionising radiation prior to the administration of the nano-systems. The *in vivo* biodistribution test was done on two animal models (Balb/C mice and White

* Corresponding author: roxpopescu@yahoo.co.uk

Leghorn chick embrios) and proved the biocompatibility of the doxorubicin-functionalized magnetite nanoparticles with living structures.

Keywords: magnetite nanoparticles, anti-tumor, drug delivery systems, ionizing radiation.

References
[1] Voicu G., Crica L.E., Fufa O., Moraru L.I., Popescu R.C., Purcel G., Stoilescu M.C., Grumezescu A.M., Bleotu C., Holban A.M., Andronescu E., Magnetite nanostructures functionalized with cytostatic drugs exhibit great anti-tumoral properties without application of high amplitude alternating magnetic fields, *Rom J Morphol Embryol*, 55(2), 357-362, 2014.
[2] Popescu R.C., Grumezescu A.M., Magnetite Nanostructures with Applications in Cancer Therapy, *Current Proteomics*, 11(2), 28-138, 2014.
[3] Cole A.J., Yang V.C., David A.E., Cancer theranostics: the rise of targeted magnetic nanoparticles, *Trends in biotechnology*, 29(7), 323 – 332, 2011.

DECONTAMINATION OF URANIUM POLLUTED SOIL USING A NEW TECHNIQUE

Aura Daniela RADU[1*], Alexandru WOINAROSCHY[2], Eugenia PAN URU[1], Antoneta FILCENCO-OLTEANU[1], Mariana FLUCU [1]

[1]Research & Development National Institute for Metals and Radioactive Resources, 70 Carol I Bvd., 020917, Bucharest, Romania

[2]University "Politehnica" of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Str. 011061, building L, Bucharest, Romania

The aim of this paper has been to find a new decontamination technique for uranium polluted soil, unexpensive and efficient. This procedure is has not been realized anymore, and it uses two types of mushrooms, namely Pleurotus Ostreatus and Agaricus Bisporus. Experimental investigations were performed on three types of soils, which have been characterized in terms of particle size distribution, structure and chemical composition. For radioactive decontamination of the soil the bio-remediation technique was applied by using two species of mushrooms at temperature of $25° \pm 2°C$ in a climatic chamber for a 6 weeks period of time. Results showed that both species grew in the presence of uranium. Decontamination tests have revealed a degree of decontamination of 31% for soil 1 (sandy soil) using Pleurotus Ostreatus and 19% using Agaricus Bisporus. For soil 2 (with a large content of clay) the decontamination degree is 27% using Pleurotus Ostreatus and 16% using Agaricus Bisporus. For soil 3 decontamination degree using both species had intermediary values.

Keywords: soil, uranium, decontamination, mushrooms, mycoremediation

Reference
[1] Ali H., Khan E., Anwar Sajad M., Phytoremediation of heavy metals—Concepts and applications, *Chemosfere*, 91(7), 869-881, 2013.
[2] Kara Y., Bioaccumulation of Cu, Zn and Ni from the wastewater by treated Nasturtium officinale, *Int. J. Env. Sci. & Techn.*, 2(1), 63-67, 2005.
[3] Arora M., Kiran B., Rani S., Kaur A., Mittal N., Heavy metal accumulation in vegetables irrigated with water from different sources, *Food Chem.*, 111(4), 811-815, 2008.
[4] Choudhury H., Mudipalli A., Potential considerations & concerns in the risk characterization for the interaction profiles of metals, *Indian J. Med. Res.*, 128, 462-483, 2008.
[5] Spergel D. N., Bean R., Doré O., Nolta M. R., Bennett C. L., Dunkley J., Hinshaw G., Jarosik N., Komatsu E., Page L., Peiris H. V., Verde L., Halpern M., Hill R. S., Kogut A., Limon M., Meyer S. S., Odegard N., Tucker G. S., Weiland J. L., Wollack E., Wright E. L., Three-year Wilkinson microwave anisotropy probe (WMAP) observations: implications for cosmology, *The Astroph. J. Suppl. Series*, 170(2), 377-408, 2007.

---

[*] Corresponding author: daniela_aura_radu@yahoo.com

COMPARATIVE STUDY ON α AND s-PINENE COMPOSITION OF VARIOUS VOLATILE OILS

Anca Daniela RAICIU[1], Mariana POPESCU[1*],   tefan MANEA[1], Ovidiu DIMA[2]

[1]S.C. HOFIGAL EXPORT-IMPORT S.A., Intrarea Serelor street, no.2, district 4, 042124, Bucharest, Romania
[2]INCDCP-ICECHIM, 202 Splaiul Independen ei, district 6,060021, Bucharest, Romania

The study describes the composition of volatile oils obtained by steam distillation of water fir (Abies alba), pine (Pinus sylvestris), juniper (Juniperus communis), rosemary (Rosmarinus officinalis), sage (Salvia officinalis) and coriander (Coriandrum sativum) using technique of gas chromatography coupled with mass spectrometry (GC-MS). Chromatographic profile revealed the presence of volatile oil components specific to each volatile oil studied. We remark the presence of   and   -pinenen in all studied volatile oils in different concentrations.
Volatile oils studied, from green sources and rich in   ,   -pinene will be used as raw materials for creating products with anti-inflammatory, antiseptic, bronchodilators properties.

Keywords: volatile oils, gas chromatography (GC-MS), Abies alba, Pinus sylvestris, Juniperus communis, Rosmarinus officinalis, Salvia officinalis, Coriandrum sativum

References
[1] Anna Wajs-Bonikowska, Monika Sienkiewicz, Agnieszka Stobiecka, Agnieszka Maciag, *Chemical Composition and Biological Activity of Abies alba and A. koreana Seed and Cone Essential Oils and Characterization of Their Seed Hydrolates*, Chemistry & Biodiversity, Vol. 12, (3), pp. 407-418, 2015.
[2] Yong-Suk Kim, Dong-Hwa Shin, *Volatile components and antibacterial effects of pine needle (Pinus densiflora S. and Z.) extracts*, Food Microbiology, Vol. 22 (1), pp. 37-45, 2005.
[3] SALAMON, I., et al. Essential oil of common juniper (Juniperus communis L.) in Albania. In: *Proceedings of the Eighth Conference on Medicinal and Aromatic Plants of Southeast European Countries (8th CMAPSEEC) 19-22 May 2014, Durrës, Albania*. Association for Medicinal and Aromatic Plants of Southeast European Countries (AMAPSEEC) p. 239-244, 2014.
[4] Bo Li, Chendu Zhang, Liang Peng, et al., *Comparison of essential oil composition and phenolic acid content of selected Salvia species measured by GC–MS and HPLC methods*, Industrial Crops and Products, Vol. 69, pp. 329-334, 2015.
[5] Tamas, V., Bordei, N., Traistaru, G. A., Ivopol, G., Cozea, A., Shuka, L., Mersinllari, M. *Variation of essential oil content from herbs used in diet and phytotherapy, from spontaneous flora - Albania and culture flora – Romania*, Journal of EcoAgriTourism Vol. 8, No. 2, pp. 259-262, 2012.

---

[*] Corresponding author: mari.popescu@yahoo.com

BIODIESEL PRODUCTION USING A SULPHONATED ACTIVATED CARBON-BASED CATALYST

Tănase DOBRE[1], Cristina Ionela GOGOAȘĂ[1], Cristian Eugen RĂDUCANU[1*]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

In this work greener tehniques for main biodiesel products separation were studied by modelling an heterogeneous catalyst able to catalyse the used food oil transesterification with methanol in reaction conditions that were limited on purpose to match homogeneous –like process conditions.

Greener techniques and greener processes are nedeed in biodiesel industry to fix the problems associated with toxic washing operations of the final products, with the total energy consumed in stages of process that can be reduced as number by using solid catalyst and with the conflictual feedstocks that can be replaced by alternative ones.

Heterogeneous catalysed process can move the feedstock from the conflictual present one, as in vegetable oils, toward the second generation type, as in used cooking oils, yellow grease, brown grease etc. Solid catalysts are more easily to prepare to attain certain properties that allow them to catalyse processes involving feedstock with high content of free fatty acids convertible to biodiesel. The process operations number can also be reduced if the catalyst benefits by properties from acid and base components inserted in cataliyst during modelling procedure and thus catalysing simultaneously esterification and transesterification reactions of used cooking oils to yield biodiesel.

In this study an heterogenous catalyst was prepared by direct sulphonation of an activated carbon with sulfuric acid 98% followed by impregnation with a base component (potassium hydroxide) to achieve both acidic and base properties to catalyze used food oil conversion to biodiesel. The oil was prior characterised (acid numbers were studied) so the catalyst acid medium allows esterification reaction to take place.

The prepared catalyst was thermally and chemically stable and showed good catalitic activity when tested in transesterification reactions to yield biodiesel under moderate homogeneous catalyst-like reaction conditions. The highest conversion reached was 94.16% while the highest biodiesel yield reached was 92.37% at 65ºC reaction temperature, 12:1 methanol/oil molar ratio and 0.75 h reaction time.

Keywords: Heterogeneous carbon-based catalyst; biodiesel; green process.

R E F E R E N C E S
 [1] Rathore V., Newalkar B. L., Badoni R.P., Processing of vegetable oil for biofuel production through conventional and non-conventional routes, *Energy for Sustainable Development* 31, 24–49, 2016
 [2] Keera S. T., Sabagh S. M. E., Taman A.R,Transesterification of vegetable oil to biodiesel fuel using alkaline catalyst, *Fuel*, 90, 42–7, 2011.
 [3] Sharma Y. C., Singh B., Advancements in solid acid catalysts for ecofriendly and economically viable synthesis of biodiesel, *Biofuels, Bioprod. Bioref*, 5, 69–92, 2011.

* Corresponding author: cristianrdcn1@yahoo.com

[4] Lubes Z. I. Z., Zakaria M., Analysis of parameters for fatty acid methyl esters production from refined palm oil for use as biodiesel in the single-and two stage processes, *Malay J Biochem Mol Biol*,17, 5–9, 2009.

[5] Lee A. F., Wilson K., Recent developments in heterogeneous catalysis for the sustainable production of biodiesel, *Catalysis Today*, 242, 3–18, 2015.

[6] Agarwal M., Chauhan G., Chaurasia S. P., Singh K., Study of catalytic behavior of KOH as homogeneous and heterogeneous catalyst for biodiesel production, *Journal of the Taiwan Institute of Chemical Engineers*, 43, 89–94, 2012.

[7] Konwar L. J., Wärnå J., Arvela P. M., Kumar N., Mikkola J. P., Reaction kinetics with catalyst deactivation in simultaneous esterification and transesterification of acid oils to biodiesel(FAME) over a mesoporous sulphonated carbon catalyst, *Fuel*, 166, 1–11, 2016.

[8] Melero J. A., Iglesias J., Morales G., Heterogeneous catalysts for biodiesel production: current status and future challenges, *Green Chem.*, 11, 1285–1308, 2009.

[9] Shu Q., Gao J., Nawaz Z., Liao Y., Wang D., Wang J., Synthesis of biodiesel from waste vegetable oil with large amounts of free fatty acids using a carbon-based solid acid catalyst, *Applied Energy*, 87, 2589–2596, 2010.

[10] Devi B. P., Gangadhar K., Prashad P.S., Prashad R.N., Ind. Patent, WO 2009/016646 A1, 2009.

[11] Zhang H., Luo X., Li1 X., Chen G. Z., He F., Wu T., Preparation and Characterization of a Sulfonated Carbon-based Solid Acid Microspheric Material (SCSAM) and its use for the Esterification of Oleic Acid with Methanol, *Austin Chem Eng.*, 1, 1024, 2016.

PRACTICES FOR REDUCING EXHAUST FLUE GAS TEMPERATURE IN REFINERY FURNACES. CASE STUDY

Sînziana R   DULESCU[1*], Loredana Irena NEGOIȚĂ[1]

[1] *Petroleum-Gas University of Ploiesti, Blvd. Bucure ti, no. 39, Ploie ti, 100680, Romania*

In petroleum refineries a large quantity of hot flue gases is generated from furnaces as waste heat. If some of this waste heat could be recovered, a considerable amount of fuel could be saved. The practice of how to recover this heat depends in part on the exhaust temperature of the hot flue gases and the economics involved.

Once with flue gas evacuation occur the largest heat losses in furnaces with the loss of flue gas enthalpy. A common practice to lower flue gas enthalpy is preheating combustion air with hot flue gases (waste gases exhausted). The preheating the combustion air offers the most effective way to increase efficiency furnaces, but not the only. Heat recovery from furnace exhausted flue gas in order to produce steam and preheating process fluids as oil fractions or petroleum products with hot flue gases are other practices.

The paper presents a case study of two systems to reduce the exhaust gas temperature in a furnace from a hydrofiner unit. An oil fraction there is heated and vaporized in furnace, by taking over heat from flue gases resulting from combustion of a fuel gas. The furnace is vertical cylindrical type, and the fuel gas used is a refinery gas mixture and sulfur - free. It is equipped with air preheater placed in the convection zone, overhead the feedstock coils and before to the evacuation of combustion gases via a chimney. The preheater provide the combustion air preheating with the exhaust gases. Analyzing flue gases is calculated the excess air coefficient. The value of excess air coefficient is 1.6 and it is very high by comparing with specified values of literature to using a fuel gas. The actual version of the operating furnace was simulated with PRO/II process simulation program. Malfunctioning with a high real flow rate air makes to decrease the evacuated flue gases temperature and this fact increase the furnace efficiency. Were performed the thermal balance and technological analyze to furnace. Their aim was to estimate the thermal values and the heat transfer coefficients where with the furnace works now.

Were proposed two variants to thermal efficiency of the furnace: the first variant propose the optimise the real thermal balance and supplementary thermal flow recovery to furnace for a secondary fluid heating from unit; the second variant propose renouncing to air preheating and revamping the furnace with a heat recovery for steam. Both proposals are compared and determineted the advantages and disadvantages of choosing one or another variante. There are set out the technological and economical arguments.

Keywords: furnace, combustion, flue gases, heat recovery

---

[*] Corresponding author: marasescusinziana@yahoo.com

References

[1] Dobrinescu, D., *Procese de transfer termic i utilaje specifice*, Editura Didactic   i Pedagogic , Bucure ti, 1983.

[2] Atreya, A., A Novel Method of Waste Heat Recovery from High Temperature Furnaces, *ACEEE   Summer   Study   on   Energy   Efficiency   in   Industry*,   2007, http://pauthoring.energytaxincentives.org/files/proceedings/2007/data/papers/67_6_063.pdf

[3] Andrews, J., Jelley, N., Jelley, N. A., *Energy Science: Principles, Technologies, and Impacts*, Oxford University Press, United Kingdom, 2013.

CONSTANTIN CALISTRU (1916- 2006): A FOUNDER OF THE *CHEMICAL PROCESS ENGINEERING* IN ROMANIA

Ilie SIMINICEANU[1*]

[1] *"Gh. Asachi" Technical University of Ia i, Department of Chemical Engineering, Iasi, & ASTR*

Today, the academic Chemical Engineering includes three basic disciplines: (I) Physical Unit Operations based on transport phenomena, (II) Chemical Reaction/ Reactor Engineering (CRE), and (III) Process Systems Engineering (PSE). The first was created by George Davis (1850- 1907) who published Chemical Engineering Handbook (1901) in Manchester. The second was officially created at the European Congress of Chemical Engineering in Amsterdam (1957). The term Chemical Reaction Engineering has been coined by Dirk Van Krevelen [1]. The third branch, PSE, was pioneered by Roger Sargent from Imperial College since 1964, and developed by Dale F. Rudd in his textbook Strategy of Process Engineering (1968).

Constantin Calistru has been the head of the chair of Inorganic Chemical Technology of the Industrial Chemistry Faculty in Iasi since 1948 till 1982, and the Dean of this faculty (1952- 1967). Independently of Van Krevelen, he defined the chemical unit operations/ chemical processes which include chemical reaction as well as other transformation and transport phenomena. Each unit chemical process has a specific macro- kinetic mechanism. He presented the theory of unit chemical operations at the International Congress of Industrial Chemistry, Bruxelles, 1966 [2]. He further developed experimental methods and mathematical models for the most important industrial processes of inorganic industry, and published the first monograph of this new discipline in 1971 [3]. In addition, he initiated and organized a national symposium on the subject, with the support of the factories in Roznov and Savinesti (Simpozionul National de Ingineria Proceselor Chimice, Piatra Neamt, 1973, 1978, 1983, 1988, 1993, 1998). He also directed over twenty PhD theses in the field. Some of the disciples became professors and PhD directors. The Academic Genealogic Tree of Professor Calistru has already four generations.

Keywords: unit chemical process, macro-kinetic mechanism, rate determining step, mathematical modeling, reactor design.

References
[1] Peppas N.A. (Editor), *One Hundred Years of Chemical Engineering*, Kluwer Acad Publ, New York, 1989, p 149.
[2] Calistru C., *Compt Rend. XXXVI Congres Internat. de Chimie Industrielle*, Bruxelles, 1966.
[3] Calistru C., *Tehnologia substantelor anorganice, Partea I: Ingineria proceselor chimice*, Edit. Didactic i Pedagogic , Bucure ti, 1971.

[*] Corresponding author: ilie.siminiceanu@tuiasi.ro

MODELING AND SCALE- UP OF A GROUND WATER DENITRIFICATION PLANT BY ION EXCHANGE

Ilie SIMINICEANU[1*], Adriana BURLACU[2]

[1] *"Gh. Asachi" Technical University of Ia i, Department of Chemical Engineering, 73 Bd. Acad Dimitrie Mangeron, RO- 700050 Ia i*
[2] *ABA Prut- SGA Botosani, str. Nicolae Iorga 37*

Several ground water sources in the rural areas of the Botosani county have nitrate concentrations approaching the WHO's maximum acceptable concentration (MAC) of 50 mg NO_3^-/L. The macrokinetic mechanism of the ion exchange is rather complex, as shown bellow:
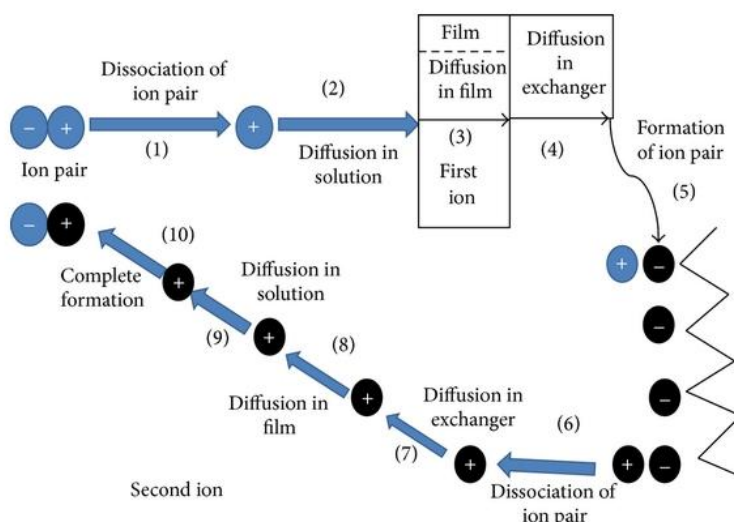
Our previous kinetic measurements have shown that the rate of water denitrification by ion exchange was determined by the two diffusion steps of the counter ions: film diffusion and/ or particle diffusion. The film diffusion may prevail when the system is characterized by the following properties: I. high concentration of fixed group; II. low concentration of ions in water; III-small particle size; IV-large film thickness or poor agitation.

The main objective of this work was to scale- up the laboratory data in order to design a full scale plant for the denitrification of drinking water by ion exchange process using a nitrate-selective resin Purolite A 520 E in order to achieve the final MAC of 50 mg NO_3^-/L. The strong base anion resin used had spherical beads of 0.3-1.2 mm particle size, in Cl^- ionic form, with a total capacity of 0.90 eq /L, apparent density of 680 kg/m^3.

Synthetic water with 100 mg NO_3^-/ L has been used for studies in a batch agitated reactor as well as in fixed bed ion exchange column. The batch results with a resin dose of 2 g/ L have shown a maximum equilibrium removal degree of 84% after 120 minutes contact time. The fixed bed column studies with a 10 cm bed height and a liquid rate of 3 m/h have shown that a constant C/C^0 could be attained in 53 hours. The data have

---

* Corresponding author: ilie.siminiceanu@tuiasi.ro

been compared with three different mathematical models: Inglezakis, Thomas, and Boyd [1]. The Boyd model considering the ion diffusion through resin pores/particle diffusion as rate determining step better predicted the experimental data ($R^2 > 0.98$).

Keywords: batch experiments, pore diffusion model, fixed- bed reactor, scale-up.

References
[1] Xu Z., Cai J.-G., Pan B.-C., *Journal of Zhejiang Univ. Science*, 14(3), 155- 176, 2013.

PROCESSES AND TECHNIQUES OF WASTE VEGETABLE OILS VIA PYROLYSIS WITH OLEFINS PRODUCTION. THEORETICAL AND EXPERIMENTAL ASPECTS

Ana-Maria SIVRIU[1*], Gheorghița JINESCU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Limitation of oil resources leads to the development of new technologies to use waste raw materials like biomass and their waste: vegetable cooking oils (rapeseed oil or sunflowers oil). Conversion of vegetable oils composed of triglycerides using pyrolisys type reactors represents a promising option for the production of renewable fuels and chemicals. The thermochemical conversion of waste vegetables cooking oils can be done by two methods: gasification and pyrolysys. Ethylene is a chemical product obtained from hydrocarbons pyrolysis. Pyrolysis of used frying oils is the best alternative of a green chemistry. The aim of the present work is to produce high yield of ethylene using waste vegetable oils from different type of uses. Following preliminary studies and literature available data, a 3- factor Box-Benken experimental study was designed for the steam cracking of waste frying vegetable oil in a micropilot plant, at atmospheric pressure, 450-550°C temperature range, contact time (1.5-2.5 s) and the mass ratio steam : raw material (0.6-1). It resulted in a reduced scheme with 13 experimental determinations for a polynomial model for which the factors were found. The waste vegetable oils is electric heated in metal tubes in the presence of steam to a temperature at which the hydrocarbon molecules thermally decomposes. The products obtained from process will be analysed using Gas-Chromatograph. The approach can be very promising and economical by using steam cracking to decrease the partial pressure of gases and to reduce coke formation.

Keywords: waste vegetable oils, triglycerides, thermochemical conversion, gasification and pyrolysys

References
[1] Lam S. Sh., Jusoh A., Chase H.A., Chong Ch.T., Progress in waste oil to sustainable energy, with emphasis on pyrolysis techniques, *Renewable and Sustainable Energy Reviews*, 53, 44-747, 2016.
[2] Billaud F., Gornay J., Coniglio L., Pyrolysis of secondary raw material from used frying oils, *Recents Progres en Genie des Procedes*, 94, 1-8, 2007.
[3] Koncsag C.I., Sterpu A.E., Dumitru A.I., Chis T., Olefins production by steam cracking of waste vegetable oil. Preliminary study, *14th GeoConference on Energy and Clean Technology*, SGEM 2014, Varna, Bulgaria, Conference Proceedings 1314-2704, vol.II, p.183-190.

---
* Corresponding author: jinescu_gheorghita@yahoo.com

GREEN SYNTHESIS OF SILVER NANOPARTICLES USING SEA BUCKTHORN EXTRACT

Ana-Alexandra SORESCU[1,2*], Alexandrina NUTA[1,3], Rodica-Mariana ION[1,2], Ioana-Raluca SUICA-BUNGHEZ[1], Cristina Lavinia NISTOR[1]

[1] *National Research and Development Institute for Chemistry and Petrochemistry – ICECHIM, 202 Splaiul Independentei Street, district 6, 060021, Bucharest,Romania*

[2]*Valahia University, Materials Dept., 13th Sinaia Alley, 130004, Targoviste, Romania*

[3]*The Romanian Academy "Stefan S. Nicolau" Institute of Virology, 285 Mihai Bravu Avenue, Bucharest, Sector 3, Zip Code 030304*

In the last 10 years there has been a constant progress regarding the methods used for the synthesis of different shaped nanoparticles and especially regarding the silver nanoparticles (AgNPs) due to the well-known antimicrobial properties of silver. Different routes are available for the synthesis of AgNPs, involving both chemical and green methods.

In recent years green chemistry methods used for the synthesis of AgNPs attracted numerous researchers mainly because thse methods are cost effective, eco-friendly, easily scaled-up for large scale synthesis and they do not require the use of toxic chemicals. These methods use either different biological microorganisms or alcoholic and/or aqueous plant extracts and are constantly gaining importance over conventional chemical routes that often involve the use of hazardous chemicals.

This work presents the biosynthesis of AgNPs using aqueous extract of *Sea buckthorn* (*Hippophae rhamnoides* L.), a plant with numerous pharmacological effects (e.g.: antimicrobial, antiulcerogenic, antioxidant, anticancer, radioprotective activity, platelet aggregation, etc.). The potential capacity of *S. buckthorn* to bioreduce Ag^+ to Ag^0 was investigated by means of different spectral techniques (FTIR, UV-Vis, absorption). UV-Vis spectra were recorded at different times (0, 30, 60, 120 minutes and also 24 h after synthesis) and the results are specific for AgNPs. Also, the size of the biosynthesized AgNPs was determined by means of diffraction light scattering measurements (DLS) only to confirm that the dimensions of the obtained particles are at nanometer scale. Also, the AgNPs obtained from *S. buckthorn* aqueous extract were compared to those obtained by the chemical method that involves sodium citrate and the results are also presented.

In conclusion, a new way to synthesize AgNPs is reported by using aqueous extracts of *S. buckthorn*. The experimental results prove that AgNPs are obtained and all the physical-chemical analysis demonstrate that the compounds found in *S. buckthorn* (e.g.: tocopherols, carotenoids, flavonoids) can act both as reducing agent for Ag^+ as well as capping agent for photosynthesized AgNPs.

* Corresponding author: alexiasorescu@yahoo.com

NEW WASTE MANAGEMENT SOLUTIONS FROM MINING INDUSTRY

Gabriela STAN[1*]

[1] *Petroleum-Gas University of Ploiesti, Blvd. Bucure ti, no. 39, Ploie ti, 100680, Romania*

Waste from the extractive/mining industry is important both because of the amount and due to its high degree of contamination. However, considering all of this, the current study proposes the implementation of a new software, on the basis of the values of the physico-chemical environmental factors measured and monitored in landfills from the oil extraction industry. This, based on the collected data, could select the storage/processing processes proper to waste so that it can later be used in agriculture. Through the results presented, the advantages of using this new software solutions are:
- updating databases, measures to improve collection methods, storage and data validation;
- quantitative status update on streams and categories, quantities of hazardous waste;
- updating the categories of collected waste;
- including the results of the pilot and of full scale projects in the measures and actions proposed in continuing future planning;
- including conclusions and recommendations of pre-feasibility studies,
- promoting investments in the treatment of certain categories of waste (such as machinery used for obtaining compost of the biodegradable fraction) will lead to their elimination and the adaptation of operators for their collection and delivery;
- the need for equipment, maintenance and spare parts for the collection, treatment and disposal infrastructure of waste, will lead to the founding of local industrial and/or commercial enties, most likely SME (Small and Medium Enterprises).

Keywords: waste, management, mining industry.

References
[1] Panaitescu C., Onutu I., Monitoring the quality of the sludge resulted from domestic wastewater treatment plants and the identification of risk factors, *Environmental Engineering and Management Journal*, vol. 12, no. 2, p. 351-358, 2013.
[2] Panaitescu C., Bucuroiu R., Study on the composition of municipal waste in urban areas of prahova county, *Environmental Engineering and Management Journal*, Vol.13, No. 7, 1567-1571, July 2014.

---

[*] Corresponding author: gabi.stan@gmail.com

MINIMIZING THE IMPACT UPON THE ENVIRONMENT BY PROCESSING THE SLUDGE FROM WASTE WATER TREATMENT PLANTS OF WASTEWATERS

Gabriela STAN[1*]

[1] *Petroleum-Gas University of Ploiesti, Blvd. Bucure ti, no. 39, Ploie ti, 100680, Romania*

By introducing running water in households, the flow of domestic wastewater will undergo a quantum leap of about 5-6 times, which in the absence of a proper system of collection, evacuation and treatment of such water, will generate pollution in the soil, subsoil and air with water contaminants or by the decomposition of organic substances contained in these waters. This can cause epidemics of infectious diseases and unsanitary areas, which would degrade the living environment of the residents of said town. Also, only the centralized collection and disposal of these waters into the environment would help to increase pollutant content of this body of water above the permissible limits.

In the operation of a wastewater treatment plant one should consider eliminating the occurrence of accidental pollution and/or minimizing the impact on the environment. This paper proposes a study of the refurbishment of a wastewater treatment plant. Thus the line of the sludge has been modified by the processing of the excess stabilized sludge, by mechanical dehydrating it with an automatic stainless steel installation. In order to ensure the necessary conditions for the use of this sludge in agriculture after it exits the mechanical dehydration plant, it was mixed with lime powder in a screw conveyor. The mixture is then subjected to exothermic reactions to 80ºC, ensuring the sludge's/mud's sanitization or any pathogenic microorganism or parasite eggs. The paper presents comparative exeprimentale data before and after the introduction of sludge processing.

Keywords: wastewater, treatment, sludge processing.

References
[1] Panaitescu C., Onutu I., Monitoring the quality of the sludge resulted from domestic wastewater treatment plants and the identification of risk factors, *Environmental Engineering and Management Journal*, vol. 12, no. 2, p. 351-358, 2013.
[2] Panaitescu C., Bucuroiu R., Study on the composition of municipal waste in urban areas of prahova county, *Environmental Engineering and Management Journal*, Vol.13, No. 7, 1567-1571, July 2014.

---

[*] Corresponding author: gabi.stan@gmail.com

BACTERIAL CELLULOSE-ALGINATE COMPOSITES FOR ACTIVE COMPOUNDS RELEASE

Anicuța STOICA-GUZUN[1*], Luminița FRIGESCU[1], Marta STROESCU[1], Iuliana JIPA[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Bacterial cellulose is a well-known microbial biopolymer which displays unique properties described largely in literature [1]. Among them must be mentioned high hydrophilicity, a very fine network structure and the possibility to be compounded with many biopolymers such as alginate. Alginate is also a known polysaccharide used in drug delivery systems or for food applications. It is also biocompatible and biodegradable and being extracted from algae's have a reasonably price [2].

Bacterial cellulose-alginate composites were fabricated by casting method and subsequent crosslinked with $CaCl_2$. To study the release properties of the composite films cinnamaldehyde was used as model flavour in our experiments. The obtained composites were characterized by Fourier transform infrared spectra (FTIR). The swelling behaviour of the composites was also studied. Cinnamaldehyde release was influenced by BC content and by crosslinker concentration.

Keywords: bacterial cellulose, sodium alginate, cinnamaldehyde, release

References
[1] Esa F., Tasirin S. M., Rahman N. A., Overview of Bacterial Cellulose Production and Application, *Agriculture and Agricultural Science Procedia*, 2, 113 – 119, 2014.
[2] Chiaoprakobkij N., Sanchavanakit N., Subbalekha K., Pavasant P., Phisalaphong M., Characterization and biocompatibility of bacterial cellulose/alginate composite sponges with human keratinocytes and gingival fibroblasts, *Carbohydrate Polymers*, 85, 548–553, 2011.

---

[*] Corresponding author: anicuta_s@yahoo.com, astoica.upb@gmail.com

ABSORBENT FOOD PADS CONTAINING BACTERIAL CELLULOSE

Marta STROESCU[1*], Anicuța STOICA-GUZUN[1], Andreea BUTURUGA[1], Alexandra MOCANU[1], Gabriela ISOPENCU[1]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Meat and poultry contain liquid and juices which must be removed when these products are packaged within a plastic wrapped tray. For this reason, many such packages contain different adsorbent materials which must have a high swelling degree. Because the liquids which are adsorbed from food products provide a medium for bacterial proliferation these adsorbent pads must have also an antimicrobial activity [1,2].

The aim of this paper is to propose a new absorbent pad for meat, absorbent fabricated from biopolymers such as: xanthan, bacterial cellulose and carboxymethyl cellulose crosslinked with citric acid. The obtained composites were characterized by Fourier transform infrared spectra (FTIR). The swelling behaviour of the composites was also studied. As antimicrobial agent potassium sorbate was used, the release of the antimicrobial agent being measured in vitro. The obtained hydrogels are promising materials which could be used in food industry having the advantage of biodegradability.

Keywords: bacterial cellulose, xanthan, carboxymethyl cellulose, potassium sorbate

References:

[1] Gouvêa D. M., Santos Mendonça R. C., Soto Lopez M. E., Batalha L. S., Absorbent food pads containing bacteriophages for potential antimicrobial use in refrigerated food products, *LWT - Food Science and Technology*, 67, 159–166, 2016.

[2] Realini C. E., Marcos B., Active and intelligent packaging systems for a modern society, *Meat Science*, 98, 404–419, 2014.

---

[*] Corresponding author: marta_stroescu@yahoo.com

SIMULTANEOUS DETERMINATION OF CAFFEIC ACID PHENETHYL ESTER (CAPE) AND FIVE POLYPHENOLS FROM ROMANIAN PROPOLIS BY RP-HPLC

Alexandru SUCIU[1,2*], T nase DOBRE[2], Iuliana CRI AN[1], Georgeta ALEXANDRU[1]

[1] *S.C. Hofigal Export Import S.A., R&D Department, Intr. Serelor street, no.2, district 4, Bucharest, Romania*
[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Propolis is a resinous byproduct of the hive formed and used by bees as a sealant, structural reinforcement and as a sterilizing agent. It has been used from ancient times as a remedy and as an embalming agent. The characteristics of propolis are due to its chemical composition consisting of over 500 compounds belonging to the polyphenols, flavonoids, terpenes, lignans, coumarins and other. Caffeic acid phenethyl ester (CAPE) is one of the important active compounds of propolis. Various studies found it possesses anti-microbial, anti-oxidant, anti-inflammatory and anti-tumor properties. This makes the quantification of CAPE from propolis an important target for making propolis-based supplements for treating/preventing various diseases.

Five types of propolis from three different locations of the country were used: Sibiu (3 types), Furcule ti and Oradea. The samples were stored in the freezer (-20 °C) before proccessing for analysis. An adapted RP-HPLC method was developed and used for quantification of CAPE, caffeic acid, chlorogenic acid, p-coumaric acid, quercetin and kaempferol.

The method showed a good separation of the peaks and a good linearity in the range used. The amount of CAPE in the samples was between 0.4 – 1.8 %. Caffeic acid, p-coumaric acid and quercetin were detected and quantified. The sum of them was in the range of 0.66 – 1.78 %. Kaempferol was also identified in the samples.

As expected, the results indicated that chemical composition of propolis varies depending on the geographical area, but also on the part of the hive it was collected from. Romania is a good source of propolis with considerable amounts of CAPE. The HPLC method used in this study is suitable for simultaneous determination of CAPE and other polyphenols from propolis.

Keywords: propolis, caffeic acid phenethyl ester, CAPE, HPLC

References
[1] Abdel‑Latif M. M., Windle H. J., El Homasany B. S., Sabra K. & Kelleher D, Caffeic acid phenethyl ester modulates Helicobacter pylori‑induced nuclear factor‑kappa B and activator protein‑1 expression in gastric epithelial cells, *British journal of pharmacology*, 146(8), 1139-1147, 2005.
[2] Cho M. S., Park W. S., Jung W.K., Qian Z. J., Lee D. S., Choi J. S., Lee D. Y., Park S. G., Seo S. K., Kim H. J., Won J. Y., Yu B. C., Choi I. W., Caffeic acid phenethyl ester

* Corresponding author: alexandru.suciu287@yahoo.com

promotes anti-inflammatory effects by inhibiting MAPK and NF- B signaling in activated HMC-1 human mast cells, *Pharm. Biol.*, 52(7), 926–932, 2014.

[3] Fitzpatrick L. R., Wang J., Le T., Caffeic acid phenethyl ester, an inhibitor of nuclear factor- B, attenuates bacterial peptidoglycan polysaccharide-induced colitis in rats, *Journal of Pharmacology and Experimental Therapeutics*, 299(3), 915-920, 2001.

[4] Garcia-Viguera C., Ferreres F., Tomas-Barberan F.A., Study of Canadian propolis by GC-MS and HPLC, *Zeitschrift für Naturforschung C.*, 48(9-10), 731-5, 1993.

[5] Gulcin I., Bursa E., ehitoglu M. H., Bilsel M., Goren A. C., Polyphenol contents and antioxidant activity of lyophilized aqueous extract of propolis from Erzurum, Turkey, *Food Chem. Tech.*, 48, 2227–2238, 2010.

[6] Huang S., Zhang C. P., Wang K., Li G. Q., Hu F. L., Recent advances in the chemical composition of propolis, *Molecules*, 19, 19610–19632, 2014.

[7] Jang M. J., Sheu S. R., Wang C. C., Yeh Y. L., Sung K. H., Optimization analysis of the experimental parameters on the extraction process of propolis, *Proceedings of the International MultiConference of Engineers and Computer Scientists*, 2, 18-20, 2009.

[8] Lin H. P., Lin C. Y., Huo C., Hsiao P. H., Su L. C., Jiang S. S., Chan T. M., Chang C. H., Chen L. T., Kung H. J., Wang H. D., Caffeic acid phenethyl ester induced cell cycle arrest and growth inhibition in androgen-independent prostate cancer cells via regulation of Skp2, p53, p21Cip1 and p27Kip1, *Oncotarget*, 6(9), 6684, 2015.

[9] Lin H. P., Lin C. Y., Liu C. C., Su L. C., Huo C., Kuo Y. Y., Tseng J. C., Hsu J. M., Chen C. K., Chuu C. P., Caffeic Acid phenethyl ester as a potential treatment for advanced prostate cancer targeting akt signaling, *Int. J. Mol. Sci.*, 14, 5264–5283, 2013.

[10] M rghita L. A., Dezmirean D. S., Drâgl F., Bobi O., Caffeic Acid Phenethyl Ester (CAPE) in Romanian Propolis, *Bulletin of University of Agricultural Sciences and Veterinary Medicine Cluj-Napoca, Animal Science and Biotechnologies*, 71(2), 111-4, 2014.

[11] Nomura M., Kaji A., Ma W., Miyamoto K., Dong Z., Suppression of cell transformation and induction of apoptosis by caffeic acid phenethyl ester, *Mol. Carcinog.*, 31, 83–89, 2001.

[12] Omene C. O., Patel M., IllaBochaca I., Barcellos-Hoff M. H., Caffeic acid phenethyl ester (CAPE) reverses aggressive breast cancer in the radiation chimera model, *Cancer Research*, 76(14 Supplement), 5247, 2016.

[13] Pascual C., Gonzales R., Torricella R. G., Scavenging action of propolis extract against oxygen radicals, *J. Ethnopharmacol.*, 41, 9–13, 1994.

[14] Sawaya A., Cunha I., Marcucci M., Analytical methods applied to diverse types of Brazilian propolis, *Chem. Cent. J.*, 5927, 1–10, 2011.

[15] Simone-Finstrom M., Spivak M., Propolis and bee health: the natural history and significance of resin use by honey bees, *Apidologie*, 41(3), 295-311, 2010.

[16] Sud'ina G. F., Mirzoeva O. K., Pushkareva M. A., Korshunova G. A., Sumbatyan N. V., Varfolomeev S. D., Caffeic acid phenetyl ester as a lipoxygenase inhibitor with antioxidant properties, *FEBS Lett.*, 329, 21–24, 1993.

[17] Tang C., Sojinu O. S., Simultaneous determination of caffeic acid phenethyl ester and its metabolite caffeic acid in dog plasma using liquid chromatography tandem mass spectrometry, *Talanta*, 94, 232-9, 2012.

[18] Wu J., Omene C., Karkoszka J., Bosland M., Eckard J., Klein C. B., Frenkel K., Caffeic acid phenethyl ester (CAPE), derived from a honeybee product propolis, exhibits a diversity of anti-tumor effects in pre-clinical models of human breast cancer, *Cancer Lett.*, 308, 43–53, 2011.

[19] Yang J. W., Jung W. K., Lee C. M., Yea S. S., Choi Y. H., Kim G. Y., Lee D. S., Na G., Park S. G., Seo S. K., Choi J. S., Lee Y. M., Park W. S., Choi I. W., Caffeic acid phenethyl ester inhibits the inflammatory effects of interleukin-1 in human corneal fibroblasts, *Immunopharmacol. Immunotoxicol.*, 36, 371–377, 2014.

79

MAJOR TECHNOLOGIES FOR ESSENTIAL OIL LAVENDER: A SHORT COMPARATIVE OVERVIEW

Cristina ERB NESCU[1*], Aurelia-Mihaela OPRESCU[1], Daniela-Simina TEFAN[1,2], M d lina HRUBARU[3],

[1] *IPROCHIM S.A., R&D Department, Bucharest – 1*

[2] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[3]*Organic Chemistry Institute "C.D. Neniţescu" of the Romanian Academy, Bucharest*

Lavender is the most used essential oil in the world. The health benefits of lavender essential oil include its ability to eliminate nervous tension(insomnia, anxiety, migraines, headaches, depression, nervous tension, emotional stress, etc.), relieve pain (tense muscles, muscular aches, rheumatism, sprains, backache and lumbago), disinfect the scalp and skin (acne, hair loss, etc.), enhance blood circulation (coronary circulation, hypertension, etc.) and treat respiratory problems (throat infections, flu, cough, cold, asthma, sinus congestion, bronchitis, whooping cough, laryngitis, and tonsillitis, etc.), digestion (stimulates the production of gastric juices and bile, thus aiding in the treatment of indigestion, stomach pain, colic, flatulence, vomiting and diarrhea) (http://everything-lavender.com/index.html).

There are five main types of lavender, among which Lavandula angustifolia (English lavender) and Lavandin are the most recommended species for essential oils extraction (Whiriskey & McCarthy, 2006). An important part of all existing technologies is lavender harvesting and its preparation prior to oil extraction, which must follow strict prescriptions in order to obtain a high quality essential oil.

The most industrially applied, efficient and recommended lavender oil technologies are: steam distillation (SD), hydro-distillation (HD), supercritical fluids extraction (SFE), solid phase micro-extraction (SPME) and solvent-free microwave assisted extraction (SFME). As a general rule, the innovative technologies (SFE, SFME and SPME) represent a very promising route, being significantly more environmental friendly and rapid than conventional ones. A third route is represented by the so-called "hybrid technologies", i.e. a combination between conventional and innovative processes. Among these hybrid technologies, mainly the ones using microwaves and ultrasounds have been the most used for lavender oil extraction. However, the main technological constraint is the use of non-corrosive materials (stainless steel or glass) for the reactor and any other necessary equipment (Rombaud et al., 2014). Moreover, the final product quality must comply with the essential oils standards in force, namely ISO/DIS 3054.

Keywords: *Lavandula angustifolia*, lavandin, lavender oil, supercritical carbon dioxide extraction, steam distillation

---

[*] Corresponding author: crst28@gmail.com

References

[1] URL: http://everything-lavender.com/index.html

[2] Whiriskey J., McCarthy P., Lavender Production, Fact Sheet no. 52, Teagasc, Mellows Development Centre, Ireland, 2006.

[3] Rombaut N., Tixier A.S., Bily A., Chemat F., Green extraction processes of natural products as tools for biorefinery, Biofuels, Bioproducts & Biorefining, 8, 530-544, 2014.

BIOGAS FROM ALGAE A NEW PERSPECTIVE TO REDUCING THE NATURAL WATER POLLUTION AND REDUCING EXHAUSTED GREENHOUSES

Daniela Simina TEFAN[1,3] *, Nicolae SDRULA[2], Cristina ORBECI[1,3], Cristina ERB NESCU[3]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[2] *ABR 19-21 M. Eminescu Street, Bucharest 1, Romania*

[3] *IPROCHIM S.A. 19-21 M. Eminescu Street, Bucharest1, Romania*

The work underlines the importance of biogas producing in the current politic-economic context, when fossil methane became uncertain to be reasonable purchased from free market. At the same time, talking in account that the raw materials, conducting to biogas, proceed basically from biomass or other organic matters, which mostly suffer a non-controlled field natural degradation, the valorization of such resources means diminishing of greenhouse exhausting, i.e. positive impact on environmental protection. The biogas produced from algae presents many benefits on environmental protection. Algae bloom is an indicator of natural water pollution, determining eutrophication through nitrogen excess. The growing and harvesting of algae remove nutrients from water and can be used for reducing of the eutrophication and for water cleaning.

The paper takes in account the state of the art regarding applied technologies of biogas, obtaining from algae, and its advantages and disadvantage, technical and economical performances compared with other technologies. Specific biogas production from different microalgae varies between 287 and 611 L/kg VS (volatile substance) similar with the best performing substrate used for biogas production [1].

The problems regarding biogas production are determined by the high contents of sulphur, sodium chloride, heavy metals and nitrogen from protein (the ration C/N for most algae is lower than 15 comparative with optimal range 15 - 25), that inhibit the algae biodegradation. Co-digestion with manure and other vegetable wastes leads to increasing of biodegradation yield [2].

The advantages regarding algae utilisation represent the low content of lignin, compound that reduces the yield of biogas production.

The benefits obtained by using algae for biogas production are multiple, including cleaning of the surface waters (lakes, see, lagoons, etc.) by nitrogen and sulfur compounds consumption, fixing of carbon dioxide from the atmosphere as biomass and producing energy (heat and power), thereby reducing consumption of fossil fuels and reducing greenhouse gases and their effects.

Keywords: energy, biogas production, eutrophication, algae biodegradation, anaerobe fermentation, carbon dioxide capture, reducing greenhouse gases.

---

* Corresponding author: simina_stefan_ro@yahoo.com

References

[1] Murphy J., Drosg B., Allen E., Jerney J., Xia A, Herrmann C., *A Perspective on algal biogas*, 10-18, 2015.

[2] Nicolik V., *Producerea si utilizarea biogazului pentru obtinerea de energie*, 5-12, 2006.

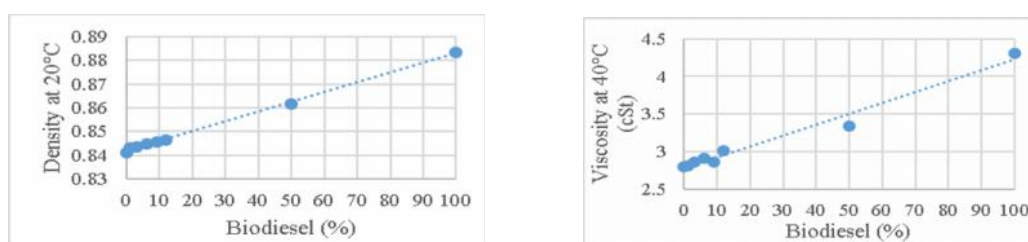# CORRELATIONS BETWEEN BIODIESEL PERCENTAGE AND DIESEL FUEL PROPERTIES

andru TEFAN[1*], Diana CURSARU[1], Ion ONUȚU[1], Dorin St nic EZEANU[1]

[1] *Petroleum-Gas University of Ploiesti, Blvd. Bucure ti, no. 39, Ploie ti, 100680, Romania*

Biodiesel is a ecological and biodegradable fuel which is currently used in Diesel fuel production, up to 5-7%, of the total final blend.[1] From a chemical point of view, biodiesel is a mixture of methyl and ethyl esters, obtained after the transesterification of triglycerides from vegetable oils. It is well known that the properties of biodiesel are slightly different from the properties of diesel fuel, and therefore the mixing ratio of these two products will decisively influence the chemical characteristics of the final product. The purpose of this study is to establish and to find a way to predict, through correlation equations, how biodiesel percentage influences the properties, density and viscosity, of the final product.

Keywords: linear regression, biodiesel-diesel blends, correlation equations.

The transesterification reaction was performed at 50°C, using corn oil and methanol (molar ratio oil: methanol= 1:3) while being stirred vigorously for 2 hours and in the presence of KOH as catalyst. In this study it was used a hydrotreated diesel fuel, taken from a Romanian oil refinery. The methyl esters were blended with the diesel fuels at 0%, 1%, 3%, 6%, 9%, 12%, 50% and 100%, in order to determine the correlation equations. Using the obtained results, a graphic representation was possible, which reveals the densies and viscosities variation, in correlation with the biodiesel percentage. The results are represented in the figures down below.

Using linear regression, two correlation equations were determined from the graphics. The equations shows how the biodiesel percentage has an impact on the two properties chosen for this study: density and viscosity. The determined equations are presented down below, formula 1 corresponding to density and formula 2 to viscosity, both being first order algebraic equations.

$$\text{Density}_{\text{blend}} = 0.0004 \cdot X + 0.8419$$

$$\text{Viscosity}_{\text{blend}} = 0.0145 \cdot X + 2.7842$$

* Corresponding author: sandru0318@gmail.com

where X represents the biodiesel percentage in the final blend.

Since the difference between the calculated values and the measured ones doesn't exceed the relative error, it is safe to say that the two correlation equations return a valid and reliable result regarding the influence of biodiesel percentage on density and viscosity. Due to the different types of biodiesel, these correlation equations are only valid for this type of biodiesel, obtained from corn oil, using the same steps as above.

References

[1] Tesfa B., Mishra R., Gu F., Powles N., *Prediction Models for Density and Viscosity of Biodiesel and their Effects on Fuel Supply System in CI Engines*, Renewable Energy, 35 (12), pp. 2752-2760, 2010.

ASSESSMENT OF MOLECULAR DESCRIPTORS FOR n-METHYLGLYCINE USING SOFTWARE APPLICATIONS

Amalia   TEFANIU[1*], Florinela SÎRBU[2], Cristina Silvia STOICESCU[2], Valeria Gabriela SAVOIU[1]

[1]*National Institute for Chemical - Pharmaceutical Research and Development - Bucharest, 112 Vitan Av., 031299, Bucharest, Romania*

[2]*Institute of Physical Chemistry Ilie Murgulescu of the Romanian Academy, Bucharest, Romania*

In order to supplement our experimental data concerning thermophysical properties for n-Methylglycine [1], a computational study using Spartan'14 software Wavefunction, Inc. Irvine CA USA was conducted on its 3D optimized structure as CPK model (ball-and-spoke). Conformational analysis was performed to find the more stable conformer, presenting the energy minima and optimized geometry. Structure dependent indicators: the octanol-water partition coefficient (logP), the number of hydrogen bond donors (HBDs) and acceptors (HBAs), polarizability, HOMO-LUMO gap, dipole moment, no. of tautomers and conformers, were reported. In addition, properties obtained from a space - filling model that are particularly valuable in QSAR type analyses have been calculated: area, volume, polar surface area (PSA), ovality. Their values were obtained using Hartree-Fock method [2], in vacuum and in water for equilibrium geometry at ground sate of the studied compound. Results have been interpreted in terms of electronic effects, molecular deformability, steric factors and reactivity, aiming to achieve a complex structural analysis.

Keywords: n-Methylglycine, molecular descriptors

References
[1] Gheorghe I., Stoicescu C., Sirbu F., Partial molar volumes, isentropic compressibilities, and partial molar expansibilities of N-Methylglycine and D-Glucose in aqueous environments at temperatures between (298.15 and 323.15) K, *Journal of Molecular Liquids*, 218, 515-524, 2016.
[2] Hehre W. J., Radom L., Schleyer P.V.R., Pople J.A., *Ab Initio Molecular Orbital Theory*, Wiley, New York, 1985.

---

* Corresponding author: astefaniu@gmail.com

ELECTROCHEMICAL CHARACTERIZATION OF SOME PYRROLO[1,2-C]PYRIMIDINES DERIVATIVES

Marian-Laurențiu TATU[1], Emilian GEORGESCU[2], Marcel-Mirel POPA[3,4], Eleonora-Mihaela UNGUREANU[1*]

[1]*Department of Inorganic Chemistry, Physiscal Chemistry and Electrochemistry, University "Politehnica" of Bucharest, Gh. Polizu 1-7, 011061, Bucharest, Romania*

[2]*Research Center Oltchim, Uzinei Street 1, 240050, Ramnicu Valcea, Romania*

[3]*Romanian Academy, Institute of Organic Chemistry "C. D. Nenitescu", Spl. Independentei, 202B, 060023-Bucharest, 35 P.O. Box 108, Romania*

[4]*Department of Organic Chemistry, University "Politehnica" of Bucharest, Gh. Polizu 1-7, 011061, Bucharest, Romania*

The electrochemical characterization of some pyrrolo[1,2-c]pyrimidines derivatives was done by cyclic voltammetry, differential pulse voltammetry and rotating disk electrode at different concentration. This study was performed in tetrabutylammonium perchlorate in acetonitrile as supporting electrolyte in a three electrode cell. Modified electrodes were obtained by cyclic voltammetry at different potentials or by controlled potential electrolysis (CPE) at different potentials and charges.
The obtained results suggest that the studied compounds are promising candidates for future practical applications.

Keywords: cyclic voltammetry, differential pulse voltammetry, rotating disk electrode, controlled potential electrolysis

---

* Corresponding author: em_ungureanu2000@yahoo.com

SIMULATION OF A TWO-STAGE ULTRAFILTRATION PROCESS FOR SEPARATING BIOMOLECULES FROM MICROALGAE

Bogdan TRIC [1,2*], T nase DOBRE[1], Gholamreza DJELVEH[3], Raluca OMOGHI[2]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[2] *The National Institute for Research & Development in Chemistry and Petrochemistry (ICECHIM), 202 Spl. Independentei, 060021, Bucharest, Romania*

[3] *Pascal Institute UMR 6602 - CNRS/UBP/SIGMA, axe GePEB, 4 Avenue Blaise Pascal, TSA 60206, 63178 Aubière, France.*

Algae (especially microalgae) are an abundant source of HVAB (high value added biomolecules) such as antioxidants, pigments, polyunsaturated fatty acids, polysaccharides and proteins which are or could become a sustainable feedstock for applications in pharmaceuticals, nutraceuticals or food industry. Apart from the intrinsic value of these compounds, algae are also expected to be a good feedstock for biofuels in the near future. Despite all the possible applications related to algae, their use at an industrial level is not yet achievable mainly due to the high costs related to separation and purification.

Ultrafiltration is a method which has already been employed for use in the food industry or for obtaining high purity streams ofcomplex biological entities such as viruses or proteins. Its main advantage over classical methods is that the separation does not depend on the processing temperature. Extraction of HVABs from algae takes place with good yields via this method.

The work presented in this process is concerned with modelling the separation of dissolved biomolecules originating from algae or microalgae by ultrafiltration. The model considered is based on the resistance-in-series model which also assumes the formation of a gel layer in certain conditions. The thickness of this gel layer is directly linked to the decrease of the permeate flux in time. The variables which affect directly the development of the gel layer are concentration and transmembrane pressure.

A one stage ultrafiltration unit is analyzed first. The predictions of the model are compared with experiments described in literature. Following this, a two-stage setup with two ultrafiltration units arranged in series is modelled mathematically and its predictions are presented. This setup is proposed for obtaining at the end of the operation one batch concentrated in high molecular mass biomolecules and another one concentrated in medium-sized biomolecules.

Keywords: ultrafiltration, protein, algae, resistance-in-series

References

[1] Vincent-Vela M.C., Cuartas-Uribe B., Álvarez-Blanco S., Lora-García J., Analysis of an ultrafiltration model: Influence of operational conditions, *Desalination*, 284, 14-21, 2012.

* Corresponding author: trica.bogdan@gmail.com

[2] Marcati A., Ursu A. V., Laroche C., Soanen N., Marchal L., Jubeau S., Djelveh G., Michaud Ph., Extraction and fractionation of polysaccharides and B-phycoerythrin from the microalga Porphyridium cruentum by membrane technology. *Algal Research-Biomass Biofuels and Bioproducts*, 5, 258-263, 2014.

BIOCOMPATIBILITY STUDY OF A METALLIC MATERIAL USED IN PROSTHETIC DENTISTRY

Graziella L. TURDEAN[1*]

[1] *"Babes-Bolyai" University, Faculty of Chemistry and Chemical Engineering, Department of Chemical Engineering, Research Center in Electrochemistry and Non-conventional Materials, 11 Arany Janos str., RO-400028 Cluj-Napoca, Romania*

In order to select a material for dental application, it is necessary to emphasize that the choice of material depends on various factors like: corrosion behavior, mechanical properties, cost, availability, biocompatibility, and aesthetic values. The corrosion behavior of metallic materials for dental applications usually is the most important property because of biocompatibility and cytotoxicity of the products generated by the corrosion process. Metal alloys are extensively used materials in prosthetic dentistry for implants and restorations due to easily cast into desired thinner shapes viz. crowns, bridges, fixed or removable partial dentures without losing the rigidity. For these purpose, they must have different properties as: high durability and good mechanical properties, good osseointegration, excellent corrosion resistance and biocompatibility in biological fluids and high resistance/weight ratio. Also, the performances of any materials (ceramics, metallic and/or alloys) placed in the oral environment should be evaluated using artificial saliva [1-2]. Most dental materials suffer corrosion in the oral cavity, except the noble metals. The resistance to corrosion of the majority of dental metals and alloys is due to the formation of a passive and protective film on their surface [3].

The aim of the study was to investigate by electrochemical techniques the resistance to corrosion and the related biocompatibility properties (resistance to corrosion induced by artificial saliva) of two alloys (Cr-Ni and Co-Cr) commercially available in the market for dental casting. Potentiodynamic polarization curves of alloys samples were obtained by varying the applied potential from -1 V to 1 V with a potential scan rate of 1 mV/s, in view to identify their active-passive behavior. Open circuit potential (OCP) measurements showed that the potential values increased with immersion time in artificial saliva, which proves a passivation process occurring to the studied alloys. The electrochemical impedance spectroscopy measurements allowed the estimation of the values of the resistance to corrosion of the studied alloys and their comparison with data from literature.

The biocompatibility properties expressed as resistance to corrosion induced by artificial saliva, recommend this dental materials as resistant in aggressive natural media.

Keywords: alloys, dental materials, electrochemical methods, biocompatibility

---

[*] Corresponding author: gturdean@chem.ubbcluj.ro

References

[1] de Queiroz G. M. O., Silva L. F., Ferreira J. T. L., Gomes J. A. C. P., Sathler L., *Braz. Oral Res.*, 21(3), 209-215, 2007.

[2] Qiu K.J., Lin W.J., Zhou F.Y., Nan H.Q., Wang B.L., Li L., Lin J.P., Zheng Y.F., Liu Y.H., *Materials Science and Engineering C*, 34, 474–483, 2014.

[3] Rodríguez-Díaz R. A., Ramirez-Ledesma A. L., Aguilar-Mendez M. A., Uruchurtu Chavarin J., Hernández Gallegos M. A., Juarez-Islas J A, *Int. J. Electrochem. Sci.*, 10, *7212 – 7226*, 2015.

SIMULATION OF REACTIVE DISTILLATION PROCESS FOR ENHANCING THE OCTANE NUMBER OF GASOLINES

Olga Valerica ȚAGA (SĂPUNARU)[1*], Mihaela BRÂNZEI[2], Silviu PASCU[2], Gheorghița JINESCU[1], Claudia Irina KONCSAG[2]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

[2] *Ovidius University of Constanta, 124 Mamaia Street, Constanta, 900527, Romania*

Following an experimental study on the olefins etherification with alcohols in the FCC gasoline, encouraging results were obtained with octane number of the gasoline increasing. It was an option to perform a complete experimental work in order to find the optimum parameters, but this requires a lot of experimental data and the octane number determination is an expensive analysis. With the help of gas chromatography, the composition of the feed gasoline was found. This constituted the start of simulations in CHEMCAD. For the simulation, compounds not found in the component database were created: iso-alkanes, cyclo-olefins and also oxygenated compounds. The hydrocarbons were treated as pseudo-components and the oxygenated compounds with UNIFAC group data. The flow-sheet mimicking the pilot plant was built in unit operations. The etherification with four alcohols (methanol, ethanol, isopropanol and 1-butanol) was studied; the azeotropes formed were identified as the cause of specific distribution of components between the top and the bottom of the fractionation column. The simulations in ChemCad led to the optimal parameters and the right position of the reaction zone in the column, in each case.

Key words: olefins etherification, gasoline octane number, flow-sheet, process simulation, reactive distillation

References

[1] Branzei M., Țaga (Săpunaru) O. V., Koncsag C. I., Influence of azeothopy on the etherification in situ of FCC gasoline, *Chimia 2016*, 26-28 May Constanta, Book of abstracts, PD4, p.67

[2] Țaga (Săpunaru) O. V.*,* Pascu S*,* Brânzei M., Koncsag C. I., Jinescu G., Augmenter l'octane de l'essence par etherification in situ, 9-eme Colloque Franco-Roumain de chimie appliquee, *CoFroCA 2016*, 28 June-2 July, Clermont-Ferrand, Book of abstracts, p.191

---

[*] Corresponding author: olgutasapunaru@yahoo.com

PODANTS WITH AZAHETEROCYCLES SKELETON AND THEIR COORDINATION COMPLEXES WITH M^{2+}

Violeta VASILACHE[1,2*], Dorina MANTU[1], Vasilichia ANTOCI[1]

[1]"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry; CERNESIM Research Center; Bd. Carol 11, 700506 Iasi, Romania.
[2] "Stefan cel Mare" University Suceava, Faculty of Food Engineering, Str. Universitatii 13, Suceava, Romania.

Azaheterocyclic derivatives are widely discussed nowadays for their applications in optoelectronics (fluorescent derivatives, chemosensors, logic gates), agriculture (growth regulators, pesticides, insecticides), ionic liquids, etc.

Within this work we present the synthesis and characterisation of a M^{2+} [(Zn (II), Co(II), Cu(II), Ni(II), Pb(II)] coordination complexes based on podants with azaheterocycles skeleton. We chose as podants azaheterocycles, having in the same molecule π–deficient heterocycles (pyridine) and π–reach heterocycles (imidazole), with the structure described bellow. Spectroscopic (Fourier-Transformed-Infrared-Spectroscopy, fluorescence, UV-Vis absorption, NMR) and electrometric (conductometry) techniques have been used to characterize the complexes and the chelating potential of podants. X-ray are under going.
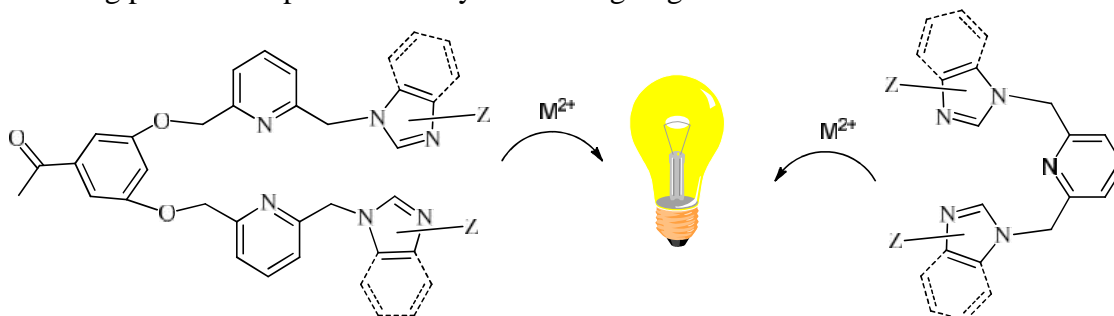
Keywords: azaheterocycles, podants, coordination, imidazole, pyridine.

References
[1] Negru A.G., Arsene C., Zbancioc A. M., Mangalagiu I. I., Olariu R. I., *Rev. Chim.-Bucharest*, 66(9), 1339-1342, 2015.
[2] Balan A. M., Miron A., Tuchilus C., Rotinberg P., Mihai C. T., Mangalagiu I. I., Zbancioc Ghe., *Med. Chem.*, 10, 476-483, 2014.
[3] Zbancioc Ghe., Florea O., Jones P., Mangalagiu I. I., *Ultrason. Sonochem.*, 19, 399-403, 2012.

---

* Corresponding author: violetaren@yahoo.com

HYBRID ORGANIC/INORGANIC NANOMATERIALS BASED ON COMPOUNDS HAVING AZAHETEROCYCLIC AND QUINONIC FRAME FUNCTIONALIZED WITH METAL NANOPARTICLES

Violeta VASILACHE[1,2*], Dorina MANTU[1], Vasilichia ANTOCI[1]

[1] *"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry; CERNESIM Research Center; Bd. Carol 11, 700506 Iasi, Romania.*
[2] *"Stefan cel Mare" University Suceava, Faculty of Food Engineering, Str. Universitatii 13, Suceava, Romania.*

The research field of nanomaterials with quinone frame and functionalized with metal nanoparticles shows an exponential growth in recent years while the field of nanomaterials with azaheterocycle frame is on borning. On the other hand, azaheterocyclic derivatives are widely discussed nowadays for their applications in medicine (drugs) and optoelectronics.

The synthesis of the hybrid organic/inorganic nanomaterials was perferformed in several steps. Initialy, we realise the synthesis of metal nanoparticles directly in a electrospinnable solution of gelatin, using the high affinity of gelatin for binding with metal ions (Ag^{1+}, Fe^{3+}, Cu^{2+} ions) and its ability to stabilize the growth of metal nanoparticles during the reduction reaction. Using specific solvent mixture and solvent volume ratio, we modify the gelatin concentration, and we realise to controll the size and shape of metal nanoparticles. Flexibilization of the nanocomposite nanofibers was achieved through a two-stage crosslinking process. The first stage of crosslinking was made in short time and at low temperature using solution of various bis-aldehydes in water which result in the formation of rigid covalent bonds between the gelatin chains. The second crosslinking stage take a longer time and was performed at room temperature using saturated solutions of different quinines with azaheterocycles skeleton. The structure of the hybrid organic/inorganic nanomaterials was investigated by FTIR, FTIR-ATR, SEM, etc.

Keywords: nanomaterials; azaheterocycles; nanoparticles; gelatine; diazine

References
[1] Tura V., Tofoleanu F., Mangalagiu I. I., Mindru T., Brinza F., Sulitanu N., Sandu I., Rileanu D., Ionescu C. J., *Optoelectron. Adv. Mater.*, 10, 3505-3511, 2008.
[2] Mantu D., Moldoveanu C., Nicolescu A., Deleanu C., Mangalagiu I. I., *Ultrason. Sonochem.*, 16, 452-454, 2009.
[3] Tura V., Hagiu B., Mangalagiu I. I*., J. Biomed. Nanotechnol.*, 6, 192-197, 2010.
[4] Mantu D., Antoci V., Mangalagiu I. I., *Infectious Disorders-Drug Targets*, 13(5), 344-351, 2013.

---

* Corresponding author: violetaren@yahoo.com

NICOLAE TECLU, THE PERPETUAL FLAME OF CHEMISTY

Dănuț-Ionel Văireanu[1*]

[1] *Politechnica University of Bucharest, Faculty of Applied Chemistry and Materials Science, Dept. of Inorganic Chemistry, Physical Chemistry and Electrochemistry*

Born in 1839 in Brasov, Nicolae Teclu belongs to the first generation of Romanian chemists who contributed greatly to the advance of scientific and technical knowledge of the second half of the nineteenth century. Better known for his gas burner, constructively and functionally superior to Bunsen's burners, Teclu graduated initially the Academy of Arts in Berlin (Die Akademie der Künste, Berlin) and came back to Romania to teach at the Romanian Secondary School (presently national college "Andrei Saguna") of Brasov. He returned to Vienna and enrolled at the Faculty of Philosophy of the University of Vienna (Universität Wien) for the purpose of studying general chemistry and analytical chemistry subjects, besides other subjects at the Imperial and Royal Polytechnic Institute in Vienna (Kaiserliches und königliches Polytechnisches Institut Wien). Appointed professor in 1971 at the Academy of Commerce in Vienna (Handelsakademie Wien), and also a reader (Dozent) at the Academy of Fine Arts in Vienna (Akademie der Bildenden Künste, Wien), Nicolae Teclu presented in many lectures held or published papers how one may successfully apply chemistry knowledge in architecture, sculpture and painting. His research and published works are very complex and of an interdisciplinary structure, Teclu succeeding a seamless combination between chemistry and fine arts, i.e.: The relations between chemistry and arts, particularly the painting (Die Beziehungen der Chemie zur bildenden Kunst, insbesondere zur Malerei), General notions about the inorganic pigments industry, apparatus for testing the quality and resistance of paper, oils used in paintings. He established various methods for reading signs printed or written on paper transformed in charred papers (bills, acts, letters). He was admitted to the Romanian Academy in 1879 and had an outstanding participation in the life of this supreme scientific forum. Although the flame of his life was extinguished in a hot summer day of 1916, Nicolae Teclu's flame is still alive in laboratories all over the world.

Keywords: Nicolae Teclu, 100 years commemoration, Romanian chemists

References
[1] Macarovici Gh. C., Schmidt G., *Nicolae Teclu*, Ed. Știinţifică, București, 1971.
[2] Iuliu Moisil, *A 70-a aniversare a naşterii chimistului român Nicolae Teclu*, Ed. Institutul de arte grafice C. Sfetea, București, 1909.
[3] Dr. Paulus Ebner, Leiter des Archivs der Technischen Universität Wien, Prof.dr.ing. Dănuţ-Ionel Văireanu, Universitatea Politehnica din București, corespondenţă personal - E2/17.02.2016
[4] Prof.dr.ing. Dănuţ-Ionel Văireanu, Universitatea Politehnica din București, Mag. Dr. Eva Schober,]a[akademie der bildenden künste wien, Universitätsarchiv der Akademie der bildenden Künste Wien, corespondenţă personal – E1/22.02.2016.

---

* Corresponding author: di_vaireanu@yahoo.co.uk

GENERAL STRATEGIES IN PRODUCT ENGINEERING

Alexandru WOINAROSCHY[1*]

[1] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

The diversity of industrial products (in many cases with close properties and with the same utilization) has a huge growth, and correspondingly, very strong market fights have evolved between producer companies. Product engineering paradigm was imposed by the fight for technical and economical product performances generated by a strong competitive market environment. Nowadays, it is far more important what and how much is sold, than what and how much is produced. The same things happened with chemical products.

Until recently, the main purpose of chemical engineering has been to obtain the lowest cost process. Even process related issues like reliability, product purity, pollution control, etc. have been ultimately translated into costs that must be minimized. In contrast, chemical product design tries to obtain the most added values for a product through enhanced product properties. This is a more complex task than a mathematical treatment to maximize profit. The profit depends in some unidentified way upon the complex set of product properties. Therefore, product engineering problems can't be solved by traditional chemical engineering approaches. Their solution requires not just additional chemical engineering approaches, but even more fundamentally.

Two general strategies for design of chemical homogeneous products are presented: a concise strategy and an extended strategy. The concise strategy consists in the next steps: identification of customer needs, generation of ideas to meet the customer needs, and the selection of the best idea. The extended strategy involves the following steps: product definition, establish of technical product requirements, identification of product performance relationships, generation of product candidate, and selection of product candidate. The two general strategies presents similarities, but there are some meaningful differences. It will be presented the details of the strategies, and the corresponding similarities and differences.

Both these strategies must be followed by process predesign, and on the base of this predesign will be performed the risk assessment and the financial analysis. The product designed by these procedures can be the starting point for mathematical optimization. Since the product that offers maximum performance regardless of costs is unlikely to be the product that offers maximum profitability, there is value in simultaneously simulating and optimizing the effects of product performance, consumer response, and microeconomics.

These straegies assumes that a homogeneous product can achieve all the required product properties. This ignores the class of chemical products known as structured products, which achieve their properties through a microstructure that is determined by the interaction of its components and the manufacturing process. Product engineering for structured products is particularly difficult, as the product and process must be designed simultaneously. In absence of a current general strategy for the design of chemical structured products, two primary approaches are possible: (1) generation and

---

[*] Corresponding author: a_woinaroschy@chim.upb.ro

systematic reduction of the number of alternative through heuristics, and (2) optimization of the set of all potential alternatives through mathematical programming.

Keywords: product engineering, design strategy, homogeneous product

References
[1] Cussler E. L., Moggridge G. D., *Chemical product design*, 2nd ed. Cambridge University Press, New York, 2011.
[2] Hill M., Chemical Product Engineering-The third paradigm*, Computers & Chemical Engineering*, vol. 33 (5), 947-953, 2009.
[3] Woinaroschy A., Raiciu A.D., *Elemente de inginerie de produs*, Ed. AGIR, Bucuresti, 2015.
[4] Gani R., *Solvent Selection through ICAS-ProCAMD*, Tutorial document, CAPEC, Technical University of Denmark, 2010.
[5] Edwards M. F., Product Engineering: Some Challenges for Chemical Engineers, *Transaction IChemE*, vol. 84, part A, 255 – 260, 2006.

EXPERIMENTAL AND MODELING OF AQUEOUS RADIOACTIVE WASTE TREATMENT BY ULTRAFILTRATION

Laura Ruxandra ZICMAN[1,3*], Elena NEACȘU[1], Felicia Nicoleta DRAGOLICI[1], Cătălin CIOBANU[1,2], Gheorghe DOGARU[1], Oana PÂRVULESCU[3], Tănase DOBRE[3]

[1] *Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH), P.O.Box MG-6, 077125 Bucharest-Magurele, Romania*

[2] *Doctoral School of Technical University of Civil Engineering of Bucharest, Lacul Tei Bdv., no. 124, Sector 2, 020396, Bucureşti, Romania*

[3] *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu Street, 011061 Bucharest, Romania*

Aqueous radioactive waste ultrafiltration was conducted using a spiral-wound polysulphonamide membrane element, 5 m^2 nominal area. The influence of process factors on its performances was experimental studied and simulated. Membrane productivity (expressed by permeate volumetric flux) and its efficiency (evaluated in terms of permeate turbidity and total suspended solids (TSS)) were measured at two values of feed flow rate, i.e., 7 and 10 m^3/h, and various levels of operating pressure (0.1-0.4 MPa), feed turbidity (1-10 NTU) and feed TSS (15-60 mg/L).

Experimental tests highlighted the following aspects: (i) permeate volumetric flux increased with an increase in operating pressure and feed flow rate as well as with a decrease in feed TSS; (ii) permeate turbidity and TSS decreased with an increase in the pressure and feed flow rate; (iii) permeate TSS increased with an increase in feed TSS; (iv) for values of feed turbidity less than 5 NTU, permeate turbidity was invariant with feed turbidity.

Mathematical models were developed in order to predict the effect of process factors on its performances as well as to scale up and optimize the process.

Keywords: aqueous radioactive waste, modeling, spiral-wound membrane, total suspended solids, turbidity, ultrafiltration.

References
[1] Bouchard C. R., Carreau P. J., Matsuura T., Sourirajan S., Modeling of ultrafiltration: prediction of concentration polarization effects, *J Membr Sci*, 97, 215-229, 1994.

---

* Corresponding author: laura.zicman@gmail.com

AUTHOR INDEX