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INTERNATIONAL WORKSHOP

"FOOD CHEMISTRY & ENGINEERING"

Book of Abstracts

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GREEN CHROMATOGRAPHIC ASSAY OF PAHs IN DIETARY SUPPLEMENTS AND FOODSTUFF

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The occurrence of polynuclear aromatic hydrocarbons (PAHs) in dietary supplements and foodstuff (especially smoked products) is a subject of a major importance with respect to the potential impact on the public health. Although the chromatographic separation of the sixteen prioritary PAHs enlisted by EPA is considered to represent an already solved analytical problem, green chromatographic approaches on the topic are still missing in the existing literature. The presented approach refers to the use of ethyl lactate as organic modifier in chromatographic separations involving PAHs. Conditions for achieving similar chromatographic retention and selectivity are discussed in detail, together with some thermodynamic consideration resulting from the van't Hoff plots.

Some sample preparation alternatives dealing with PAHs assay in difficult (fatty) matrices are also discussed. One alternative uses a silver ion loaded cation exchanger SPE material used for isolation of PAHs in vegetable oils, followed by on-line desorption and chromatographic separation. The other approach uses the unique characteristics of supercritical CO_2 to selectively extract PAHs from meat.

Last but not least, some aspects relating to the selectivity of genuine stationary phases with biphenyl chemically modified silicagel used for LC separation of PAHs are briefly highlighted.

NMR SPECTROSCOPY IN FOOD SCIENCES

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Food composition can be affected by factors like processing, storage conditions, environmental pollution, row material origin, and so on. Food materials range from homogeneous and relatively simple mixtures like oils or juices, to complex heterogeneous systems like meat or bread.

In 1960's NMR became an indispensable tool in chemistry for structure elucidation of pure compounds, and until late 1980's this remained the most important type of application. Once the high field NMR spectrometers entered the chemical community the method started to be used also for complex mixture analysis, penetrating fields like medicine or food sciences. Today we see a rather balanced use of the NMR spectroscopy between the structure elucidation of pure compounds and analysis of complex mixtures.

In addition to a presentation of the current worldwide NMR applications to foodstuff, the paper presents some successful examples from our laboratory in the fields of edible oils, fruit juices, wine, and plant metabolomics. Our interpretation approaches include both classical NMR spectra processing based on chemical shifts, integrals/intensities and multiplicities, as well as blind chemometric processing.

Acknowledgements
The author acknowledges the financial support of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project number PN-II-PT-PCCA-2013-4-0791.

MARINE BIOMASS FROM ROMANIAN BLACK SEA COAST AND SEWAGE SLUDGE AS INNOVATIVE BIOCOMPOSITE FERTILIZER

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The soils in Dobrogea area, Romania, have a variety of genetic and environmental conditions. Generally, under natural conditions, the fertility and production potential of these soils allow crop structure diversification. In the recent years, due to both climate change and human factor, the decreasing of soil fertility lead to increasing the area under degraded lands. Of genetically that most soils have loose parental material which contributes to more rapid soil degradation. The goal of this study was to obtain an ecological biofertilizer consisting of a mixture in optimal ratio between two types of residual biomass (marine biomass - algae and zoobenthos along Romanian Black Sea Coast and composting sanitized sewage sludge resulting from wastewater treatment plant of Constanta) in the aim of increasing the bonitation potential of degraded psammo-soils from Dobrogea area. The biofertilizer mixture was physical-chemical and microbiological characterized. The results obtained show the presence of organic compounds (protein, fat-soluble substances, β-carotene), carbon and nitrogenous compounds in the marine algal and zoobenthos biomass. In the sewage sludge were identified nitrogenous substances, chlorides, phosphates and a significant level of total organic substances. For the new biofertilizer, the *p*H values falls within the standardized limits of composting sewage sludge used in agriculture and a significant level of benefit organic substances, nitrogenous substances and phosphates which substantially contribute to improving the quality of poor soils, was observed. Biofertilizer composition of mineral salts (copper, zinc, manganese, iron, cobalt, nickel, lead, cadmium, mercury, aluminum) indicates regular limits in heavy metals content. Also, the presence of pathogens strains TNG, *Escherichia coli*, *Salmonella sp.*, *Staphylococcus*

sp., *Pseudomonas aeruginosa* and different species of fungi have been monitored. For the microbial charge determination, the serial dilutions method has been applied and the qualitative and quantitative identification by the colony forming units reported to the volume unit, was realized. The comparative microbiological characterization assessed that the two residual biomasses could be successfully mixed recovered in the aim to obtain a new biocomposite fertilizer with decreased bacterial charge. After biofertilizer application on psammo-soil, a tested soil low in nutrients, a slightly alkaline *p*H values, soil humus percentage and also total phosphorus, nitrogen and potassium content increased, were registered. No translocation phenomena regarding heavy metal content was observed. The results emphasize that the new biosolid composite obtained as a mixture between two residual biomasses, will offer new possibilities of the organic matter and nutrients of the sewage sludge and marine biomass, as an ecological product, a bio resource, to improve the soil quality for agriculture purpose.

EVALUATION OF ANTIOXIDANT ACTIVITY AND BIOACTIVE COMPONENTS DETERMINATION OF EUROPEAN HOPS

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The consumer's demand for the quality and safety fresh vegetables has been increasing due to the ease of intake and nutritional benefits. Epidemiological studies have correlated the consumption of bioactive ingredients with declining the incidence of several physiological threats. It is known that the amount of each compounds in vegetables have a significant impact on the quality of the foods. The bitter acids of European Hops (*Humulus lupulus*) may possess anti-inflammatory and anti-proliferative activity and the flavonoids may also have anti-proliferative properties. Hops have been characterized as a "broad spectrum" cancer chemopreventive agent in vitro studies [1]. Hops compounds have also been shown to reduce triglycerides and free fatty acid levels. It is an important source of potassium, magnesium and many micronutrients. It is also ideal for low-sodium diets which is present in small quantities. In this study, samples of hops collected at different sites in the some rivers of Ferrara country, were characterized to content of protein, lipid, mineral and we evaluated the antioxidant properties of methanolic extracts and the content of carotenoids by HPLC-UV. The samples showed a good protein content. The determination of the mineral fraction showed that hops are an excellent source of potassium and magnesium, and are ideal for low-sodium diets, which is present in small quantities. The fatty acid analysis by GC-MS shows a high percentage of polyunsaturated fatty acids, primarily linoleic and α-linolenic. The analysis of the antioxidant component highlighted a positive correlation between total phenolic content (Folin-Ciocalteu) and antioxidant capacity (DPPH assay); furthermore, it was revealed a good content of beta-carotene [2]. In all the samples analyzed, the antioxidant properties were similar but it must be considered that the functional components of hops can be affected by many factors, in particular the ripening time and the climate characteristics of the area. These results encourage further study to evaluate the potential of hops as food with health properties.

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ORGANOCHLORINE CONTAMINANTS (PCBs, DDTs, HCB AND HBDE) IN FISH FROM THE LAKE VARNA AND THE LAKE BELOSLAV, BULGARIA

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Concentrations of organochlorine compounds such as polychlorinated biphenyls (PCBs), DDT and its metabolites, hexachlorobenzene (HCB), and hexachlorobutadien (HBDE) were determined in three fish species: goby (*Neogobius melanostomus*), golden grey mullet (*Mugil auratus*) and silverside (*Atherina boyeri*). Samples were collected from the Lake Varna and the Lake Beloslav in 2014. The edible fish tissues were analyzed in order to investigate the presence of pollutants in species from the lakes near Varna city, Bulgaria and compared the results to the levels in other aquatic ecosystems. The fifteen congeners of PCBs, HCB, HCBD, DDT and its two main metabolites DDE and DDD were determined by capillary gas chromatography system with mass spectrometry detection. The OCPs levels in the wild fish were found in the order DDTs > PCBs. The other contaminants HCB and HCBD were not detected or were below the analytical detection limit. Among the pesticides, essentially only the metabolites p, p'-DDE and p, p'-DDD were found.

The concentrations of DDTs were determined from 2.66 to 17.97 ng/g wet weight and PCBs concentrations were found from 0.43 to 8.05 ng/g ww (in goby and golden grey mullet, respectively). The sum of the six Indicator PCBs did not exceed the European maximum limit 75 ng/g wet weight. The concentrations of DDTs and PCBs were found lower compared to those in similar fish species from other aquatic ecosystems.

COMPARISON OF HEAVY METAL CONCENTRATION OF SOME MARINE FISH FROM BLACK AND AEGEAN SEA

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Fish are the major part of the human diet and it is not surprising that numerous studies have been carried out on metal accumulation in different fish species. Fish also have been popular targets of heavy metal monitoring programs in marine environments because sampling, sample preparation and chemical analysis are usually simpler, more rapid and less expensive than alternative choices such as water and sediments.

Concentrations of lead, cadmium, nickel, copper, manganese, zinc, iron, chromium, total mercury and total arsenic were determined in edible part of two commercially valuable fish Greek aquaculture species Europian seabass *(Dicentrarchus labrax*) and gilthead seabream (*Sparus aurata*) purchase from Bulgarian market during 2011. The concentration of metals was measured by atomic absorption spectrophotometry (AAS). The concentration of the heavy metals in examined fish species ranged as follow: Pb 0.008– 0.013; Cd 0.0017– 0.022; Ni 0.007– 0.012; Cu 0.054 - 0.115; Mn 0.043– 0.09; Zn 0.14 – 0.15; Fe 0.17– 0.19; Cr 0.05– 0.07; Hg 0.11-0.13; As 1.6 -1.8 mg kg^{-1} wet weight, respectively.

The concentration of the heavy metals obtained from this study is compared with the results of a Black Sea bluefish (*Pomatomus saltatrix*) caught during the same year. The concentration of metals was significantly affected by the sampling site and fish species. Difference in the heavy metal concentration between Europen seabass, gilthead seabream is observed for Cu, Mn, Zn and Fe. Although, the heavy metals in the edible parts of the investigated fish were in the permissible safety levels for human uses.

VEGETABLE RESIDUES AS FEEDSTOCK FOR THE FERMENTATIVE PRODUCTION OF LACTIC ACID

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The lactic acid is a hydroxyl acid with many applications in the food, pharmaceutical, cosmetic and other chemical industries, being used as an acidulant, flavor enhancer, and preservative. Recently, the lactic acid production became more interesting because it can be used as a feedstock for the production of poly-lactic acid, a polymer involved in medical applications and in biodegradable plastics fabrication.

The lactic acid is mainly produced by the microbial fermentation, using economic resources, such as rice bran, paper sludge, green microalga, etc. The renewable materials such as lignocellulose and starch, *e.g*. from agricultural and food industry residues, represent an attractive substrate as feedstock for the production of lactic acid due to their availability and abundance.

We obtained the lactic acid by the fermentation of vegetal residues derived from apples, potatoes and bananas. We also studied the effects of fermentation condition on lactic acid production (pH, time, temperature). The concentration of the lactic acid was determined by the modified Taylor method. Our study revealed the pH dependence of the fermentation, but the optimal conditions depends on each feedstock. The processing of vegetal residues is also important for the fermentation yield. We identify the potatoes residue as proper feedstock for the production of lactic acid, in neutral medium. As well, in acidic medium, the apples residue is a suitable feedstock for the production of the lactic acid.

THERMAL EXPANSION COEFFICIENT FOR DIFFERENT VEGETABLE OILS

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In this study, value of thermal expansion coefficient was determined for six different edible vegetable oils: sunflower, corn, soya, rapeseed, olive, and palm oil. Thermal expansion coefficient indicates the changes of volume with temperature variation at constant pressure and is defined as:

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p \qquad (1)$$

where α is the thermal expansion coefficient, V is the volume, T is the temperature, and subscript p indicates constant pressure.

Thermal expansion coefficient is an important parameter for engineering calculation, and for financial reasons, taking into account that commercial transactions of vegetable oil are made on a volume basis. A higher value for the thermal expansion coefficient means less mass of oil corresponding to the same volume at higher temperature.

The thermal expansion coefficient values were calculated considering the density, as function of temperature. The density of vegetable oils was experimentally determined on an Anton Paar densimeter DMA 4500 type, in the temperature range 293.15-303.15 K at atmospheric pressure. Before the beginning of the measurement, the equipment provided with a U-vibrating measuring cell, was calibrated with doubled distilled water and dried air. The uncertainty in density measurement was ± 0.0001 $g \cdot cm^{-3}$.

The values of thermal expansion coefficient were found to be 7.40 $x10^{-4}$ K^{-1}, 7.60 $x10^{-4}$ K^{-1}, 7.85 $x10^{-4}$ K^{-1}, 8.03 $x10^{-4}$ K^{-1}, 8.06 $x10^{-4}$ $K^{-}1$, and 8.07 $x10^{-4}$ K^{-1} for the six investigated vegetable oils: rapeseed oil, olive oil, palm oil, corn oil, soya oil, and sunflower oil, respectively. The thermal expansion coefficients of sunflower oil and soya oil were the highest ones but not too different from the others, indicating some thermal behavior differences.

PHYSICO-CHEMICAL CHARACTERISATION AND BIOLOGICAL ACTIVITY OF SOME Cu(II) COMPLEXES WITH NITROGEN HETEROCYCLES AS LIGANDS

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A good biological activity such as anti-inflammatory, antimicrobial, and antitumor one was observed for some polyfunctional ligands with nitrogen donor atoms. As result several complexes with this kind of ligands derived from pyridine or pyrimidine were synthesised and some evidenced antitumor, anti-inflammatory, antimicrobial or neurological activity.

Having in view these aspects, we extended this field in synthesis of new complexes of Cu(II) with nitrogen-based heterocycles such pyridine and pyrimidine. The features of complexes have been assigned from elemental analyses, IR, UV-Vis-NIR, EPR spectra, magnetic susceptibility at room temperature as well as thermogravimetric analysis. The ligand behaves as multidentate species resulting in distorted octahedral stereochemistry in all cases.

The *in vitro* screening of the antimicrobial activity were performed against Gram positive (*S. aureus, B. subtilis*), Gram negative (*E. coli, P. aeruginosa, K. pneumoniae*) and fungal (*C. albicans*), both reference and clinical isolates multidrug resistant strains. In all cases it was evidenced that overall antimicrobial potency of ligand was enhanced upon coordination, regarding both resistant planktonic and biofilm embedded pathogenic strains. The pyrimidine derivatives exhibit a better activity concerning Gram negative strains inhibition. All species were evaluated also for influence on HEp-2 viability.

PHYSICO-CHEMICAL AND ANTIMICROBIAL CHARACTERISATION OF SOME Co(II) AND Cu(II) COMPLEXES WITH BIGUANIDE DERIVATIVES

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The increasing incidence of bacterial drug resistance imposes an improvement of the used antimicrobial drugs and also the development of new ones. In the last years the attention in this field was oriented to inorganic species considering that such compounds provide a different mechanism of action. So far, a good antimicrobial activity was observed for complexes bearing a biocation and a multidentate ligand and/or a ligand having a proved antimicrobial activity.

The biguanide derivatives fulfil both requests and in order to obtain inorganic antimicrobials new complexes of Co(II) and Cu(II) with 2-tolylbiguanide and 1,3-phenylene *bis*-biguanide were synthesised and characterised. The features of complexes have been assigned from microanalytical, IR, UV-Vis-NIR, EPR and thermogravimetric data.

The *in vitro* qualitative and quantitative antimicrobial activity assays performed against Gram positive (*S. aureus, B. subtilis*), Gram negative (*E. coli, P. aeruginosa*) and fungal (*C. albicans*) strains showed that complexes exhibited variable antimicrobial activity against Gram-negative and Gram-positive strains, both planktonic and biofilm embedded. In all cases it was evidenced that overall antimicrobial potency of ligand was enhanced upon coordination, concerning both resistant planktonic and biofilm embedded pathogenic strains. Copper (II) complexes were more active in the case of Gram negative strains.

NEW BIOLOGICALLY ACTIVE COMPLEXES WITH PYRAZOLE OR BENZIMIDAZOLE AS LIGANDS

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The coordination chemistry of pyrazole derivatives received a scant attention in the last decade although the pyrazole nucleus is thermally and hydrolytically very stable. A literature survey revealed that pyrazole derivatives possess diverse pharmacological activities such as antitumor, angiotensin-converting-enzyme (ACE) inhibitory, antimicrobial, anti-inflammatory, antiviral, anticonvulsant and antidepressant. Stable, inert, and non-toxic metal complexes containing spectroscopic active metal centers are exceptionally valuable as probes for biological systems.

Benzimidazole moiety is structurally related to purine bases and is found in a variety of naturally occurring compounds such as vitamin B_{12}. Benzimidazole derivatives exhibit a wide variety of pharmacological properties including antitumor activity and inhibition of nucleic acid synthesis. The coordination chemistry of benzimidazole derivatives was not enough studied too, despite their complexes exhibit interesting spectral and magnetic properties. Their important role in the functioning of a number of biologically significant molecules has generated further interest in these ligands.

In this context, new cobalt complexes with mixed ligands, pyrazole/benzimidazole derivatives and acrylato ions have been synthesized and characterized by chemical analysis, IR and electronic spectroscopies and by thermal analysis. Their influence on the microbial growth was assayed also.

QUALITY CONTROL OF SOME FISH PRODUCTS

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Fish is a key source of protein and essential nutrients but is also the major source of environmental metals exposure.

Aim of the study was to evaluate the quality of sprat, measuring the following parameters: alkalinity, acidity, NaCl content, moisture content, peroxide and saponification index; identification and determination of formaldehyde and hydrogen sulfide, total protein content and concentrations of Cu, Cr and Fe. Analyses were performed on four samples of sprat products: frozen, marinated, smoked and canned in oil.

The highest value for the protein content was obtained for frozen fish (11.35 %). The chromium concentrations were between 0.0001 and 0.07 mg/kg for the analyzed samples while the highest concentration of iron was obtained for canned fish oil (9.01 mg/kg).

QUALITY CONTROL OF CHOCOLATE

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According to the legend, chocolate was the food of Gods. Its main components come from fermented, crushed and roasted cocoa beans, the seeds of the tropical *Theobroma Cacao L* tree.

The dark chocolate has the smallest amount of added fats, while milk and white chocolates contain higher amounts of milk and cocoa butter than dark chocolates.

Aim of the study was to follow the evolution of quality parameters (humidity, alkalinity, acidity, pH, invert sugar, sulfur dioxide) for different types of chocolate: white, black, dark and milk. The concentration of copper, chromium and total iron by standard addition method using UV-VIS molecular spectrometry were determined. To determine whether the chocolate samples were forged, reactions to identify the gelatin and starch were carried out. The peroxide is used as an antibacterial agent in the processing of chocolate and sodium hydrogen carbonate has a regulatory role of acidity. Some reactions to identify peroxide and sodium hydrogen carbonate were carried out.

Following chemical analysis it was found that all analyzed parameters are below the maximum limits allowed by law.

COPPER AND CHROMIUM LEVELS IN CANDIES AND CANDY PACKAGES

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Various plastic materials are used in candies packaging and most of them have inorganic pigments used in inks and plastics that can contaminate the food.

Heavy metals, such as copper and chromium can pose health problems. Cr exposure is associated with cancer induction in humans.

Aim of the study was to determine the levels of Cu and Cr from candies and candy packages using the standard addition method. Samples were digested using the acid digestion and the dry ash method. Copper and chromium have been found in small quantities in candy packages and were not found in candies.

PHYSICO-CHEMICAL CHARACTERISATION OF FRESH MILK AND MILK POWDER

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Milk consumption is important in the diet of all age groups because it provides important nutrients that are essential for humans. Children are the largest consumers of milk, thus, it's very important that milk is free of toxic compounds that can be harmful for humans.

Milk powder typically contains approximately 25.2% protein, 38.1% carbohydrates, 26.2% fat, 7% ash and 3.5% water. Fat, carbohydrates and protein are important to human nutrition being excellent sources of energy.

Aim of the study was to determine the physico-chemical characteristics of 5 sample of milk powder for different stage of baby growing (0-6 months; 6 months; 10 months; 1 year; more than 2 years) and for 3 samples of fresh milk: raw cow's milk, milk trade and UHT type. The following physico-chemical properties: density, pH, acidity, the presence of acetone, enzymes, $NaHCO_3$ or antiseptics, dry substance, the ash, total fat, saponification and peroxide index, total nitrogen and protein content were determined.

Comparing the values of acidity for analyzed samples it can be concluded that the powder milk acidity value is much lower than the fresh milk. The presence of antiseptics and acetone was not identified, and amylase and peroxidase were found only in raw cow's milk. The highest protein content was found for milk powder (23.22%).

IMPACT OF CONTAMINANTS CADMIUM AND LEAD ON SOIL AND GRAPE FROM MURFATLAR VINEYARD

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Monitoring of heavy metals in fruits is an important issue with regards to human health. The plants usually translocate larger quantities of metals to their leaves rather than to their fruits or seeds. Plants can contain metallic species taken from the soil, water and air.

Heavy metal contamination in the grapes and the soil was investigated. This concept implies that there is a strong relationship between the composition of the grape and the territory of production. In order to study this link, a flame atomic absorption spectrometry (FAAS) method was applied.

The aim of this study is to quantitatively analyse the level of Cd and Pb in *Vitis vinifera* L grape fruits and soil. The grapes and the soil used in this work were purchased from the Murfatlar city, an unpolluted area. Cd and Pb were quantified by after the chemical mineralization of the samples using nitric acid and hydrogen peroxide.

It can be noticed that the values of cadmium and lead concentrations of grapes were lower than the recommendable maximum limit of these metals in fruits.

DETERMINATION OF Cu AND Zn IN SAMPLES OF GRAPE AND SOIL FROM MURFATLAR VINEYARD

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For most people, diet is the main route of exposure to trace metals, so the assessment risks of these elements to human via dietary intake is important. Under certain conditions, either essential micronutrients, such as Cu and Zn, in the environment might accumulate to a toxic concentration level, leading to ecological damages. Hence the accumulation of metals in the environment was of increasing concern due to the food safety issues and potential health risks.

The aim of this study was to analyze quantitatively the level of Zn and Cu in *Vitis Vinifera* L. grapes fruits and soil. The grapes used in this work were purchased from the Murfatlar city, Constanta, Romania. The elements: Zn and Cu were quantified by flame atomic absorption spectrometry (FAAS) after the chemical mineralization of the samples with nitric acid and hydrogen peroxide in a Digesdahl device.

It can be noticed that the values of cooper and zinc concentrations from both kind of samples (grapes and soil) were lower than the recommendable maximum limit of these metals in fruits respectively soil.

ESTIMATION OF PRESSURE DROP IN GASKET PLATE HEAT EXCHANGERS

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The calculation of pressure drop is an important part of the technological dimensioning of gasket plate heat exchangers since the power consumption for pumping is determined by the pressure loss in the equipment.

In design, the estimation of pressure drop in exchangers is made with correlations recommended in literature. All these correlations take into account the geometry of the equipment, the hydrodynamic regime and the physical properties of fluids.

The aim of this work was to select a reliable mathematical model from literature, for the estimation of pressure drop in gasket plate heat exchangers used in the vegetable oil refining industry.

Different models developed by: Kumar, Mulley, Bond and Buonapane were applied in industrial conditions. There were 6 heat exchangers of this type in an industrial plant, in different size and working with different fluids (oils with changing properties, cooling water and condensing steam).

The pressure drop values calculated with Mulley relationship and Buonapane correlation were very close and also Bond's equation gave results close to the previous but underestimated. Kumar correlation gave results far from all the others and its application will lead to oversize.

Following this comparative study we recommend the relationships of Mulley and Buonapane for the estimation of pressure drop in gasket plate heat exchangers. The Kumar correlation should be applied with caution since it results in oversisizing.

A STUDY OF THE INFLUENCE OF GAS CHANNEL PARAMETERS ON HT-PEM FUEL CELL PERFORMANCE USING FEM ANALYSIS

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Proton exchange membrane fuel cells (PEMFC) are highly efficient power generators, achieving up to 50-60% conversion efficiency, even at sizes of a few kilowatts. Comsol Multiphysics, a comercial solver based on the Finite Element Method (FEM) was used for developing a three dimensional model of a high temperature PEMFC that can deal with both anode and cathode flow field for examining the micro flow channel with electrochemical reaction. Cathode gas flow velocity influence on the cell performance was investigated at first. Polarisation curves for three different channel widths (0.8, 1.6 and 2.4 mm) and three different channel depths (1, 2 and 3 mm) were computed at a cathode inlet flow velocity of 0.06 m/s. Oxygen molar concentration at cathode catalyst layer-gas diffusion layer interface and local current density variation along the cell length were also studied for specific gas channel geometries.

RECYCLING OF POLYETHYLENE TEREPHTALATE (PET) FROM BEVERAGE WASTES BY ORGANOCATALYTIC DEPOLYMERIZATION

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Polyethylene terephtalate (PET) it is widely used in the textile and the food industry. In the last decades, the demand of PET has increased significantly for food packaging as well as bottle markets, due to its low cost of production and shock resistance. The driving consumption of PET is given also by the fact that it is environmentally friendly, but because it is not biodegradable it must be recycled. The most efficient recycling method is the metal-catalyzed glycolytic destruction of PET using mainly heavy metal salts, methodology that shows two major drawbacks: harsh reaction conditions and contamination of the glycolyzed products with heavy metals, making the product useless for food packaging. Therefore, organocatalytic glycolysis of PET wastes is more appealing and received a considerable attention lately. We present herein an improved synthetic protocol for organocatalytic glycolysis of various PET wastes through screening of various commercially available compounds. The PET glycolysis was performed in the absence of a classical organic solvent, using instead excess of EG and 5-10 % molar loading of organocatalyst, at temperature reaching maximum 190 °C. The catalytic activity was evaluated by the amount of generated bis-2-hydroxyethyl terephthalate (BHET) monomer. For a better assessment of organic catalyst efficiency the glycolysis of PET waste was performed with various glycols such us diethylene glycol, propylene glycol and isosorbide yielding some oligoesters-polyols that are used to produce polyurethane foams. Furthermore, modified organocatalyst structures were tested towards PET glycolysis in order to improve the reaction conditions as well as the catalyst loading. In addition, detailed NMR spectroscopy of both PET wastes, glycolized PET and mechanistic investigations will be presented.

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INCLUSION COMPLEXES OF NATURAL CYCLIC OLIGOSACCHARIDES

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Cyclodextrins, are most often used as hosts in different inclusion complexes. They are natural cyclic oligomers of α-D-glucose formed by the action of certain enzymes on starch. Cyclodextrines have a series of properties making them suitable as carriers: different cavity size, low toxicity, water solubility and protection of the included guest from biodegradation.

Benzimidazolium derivatives have several applications in biology, pharmacology and veterinary medicine.

A series of benzimidazolium salts bearing a *para*-halogenophenyl end group in position 3 was subjected to complexation with α- and β-cyclodextrins. Two out of the three studied compounds were leading to inclusion complexes with both cyclodextrins. For both cyclodextrins the strength of interaction with bezimidazolium ions increases in the order F<Cl<Br.

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NMR FINGERPRINTING AND DISCRIMINATION OF VEGETAL JUICES

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NMR spectroscopy is already established as a powerful analytical tool in plant research. There is an extensive literature based on NMR characterization of different plant parts (leaves, roots, fruits, etc), plant extracts or in vivo measurements of secondary metabolites.

One of the easiest ways to characterize the plants through high resolution NMR is to analyze the juice obtained by squeezing different plant components.

The paper presents a feasibility study for fast and automatic discrimination of natural and processed fruit juices. The NMR data from several juices have been subjected to statistical processing in order to develop a model for fruits discrimination based on metabolomic spectral fingerprinting.

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PRECIPITATION AND CHARACTERIZATION OF ASPHALTENES FROM ROMANIAN HEAVY AND LIGHT CRUDE OILS

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The asphaltenes are the heaviest and the most polar components in crude oils. They are soluble in toluene, but insoluble in light alkanes (n-pentane, n- heptane). The asphaltenes are a compound class with a very complex structure consisting in poly condensed aromatic rings, aliphatic chains, naphthenic rings, and heteroatoms such as nitrogen, oxygen, sulfur and trace metals (Ni, V, Fe). Asphaltenes may precipitate during crude oil processing causing transportation problems and some components may lead to catalysts deactivation affecting the cost of processing.

In this study asphaltenes were obtained by precipitating from different crude oil samples. The crude oil samples were from different regions of Romania (Ileana near Bucharest, Suplacu de Barcău, Black Sea). Crude oil samples were characterized by their main physico - chemical properties such as density, viscosity, salt content, metals and sulfur content. The precipitation and quantification of asphaltenes was performed according to ASTM D3279 method with n- heptane as solvent precipitation. Trace metals (Ni, V, Fe) and S and N content were determinated in the precipitated asphaltenes. The aim of this study was to establish a correlation between different properties of crude oils and their asphaltenes content, and between the content of heteroatoms from crude oils and asphaltenes content.

ANTIOXIDANT ACTIVITY OF SOME SPICES

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Antioxidant activity of *Rosmarinus officinalis* L. (rosemary), *Salvia officinalis* L. (sage) and *Origanum vulgare* L. (oregano) was studied.

Alcoholic extracts from these *Lamiaceae* spices were obtained by Soxhlet and ultrasounds methods. Antioxidant activity was determined by DPPH free radical scavenging spectrophotometric method and a chemiluminescence method based on luminol-Co(II)/EDTA-H_2O_2 system.

The Electron Paramagnetic Resonance (EPR) spectroscopy was used to evidence the radical species resulted by oxidation of phenolic compounds present in the plant extracts. EPR analysis of extracts has been done using DPPH free radical and 5,5-dimethyl-1-pyrroline-N-oxide (DMPO). EPR spectra of the samples were registered in two solvents with different polarity ethanol and dichloromethane.

Values of antioxidant activity determined by spectrophotometric method varied between 0.779 ± 0.035 and 2.81 ± 0.16 g gallic acid equivalents/100 g dw (dry weight) and are in concordance with the values obtained by chemiluminescence method (0.554 ± 0.0035 and 9.32 ± 0.83 g gallic acid equivalents/100 g dw).

Extraction methods do not influence significantly the antioxidant activity of extracts.

The experimental results have shown that rosemary extracts have the highest antioxidant activity, results also confirmed by EPR spectra.

CHARACTERIZATION OF SEVERAL OLEAMIDE ANALOGUES ANTI-OBESITY AGENTS BY ELECTROCHEMICAL METHODS

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Many researches are nowadays dealing with elucidating the molecular mechanism of obesity and developing new potent therapeutic agents with less secondary effects. We have synthesized oleamides analogues, similar to the natural active compounds. In this paper we present the results obtained in the study of the electrochemical profile of some oleamides, with different alkyl and aryl substituents.

The electrochemical behavior of oleamides analogues compounds was studied in acetonitrile containing tetrabutylammonium perchlorate as supporting electrolyte, using stationary or rotating glassy carbon electrodes and the processes were identified by cyclic and differential pulse voltammetry. Modified electrodes have been obtained. Electrochemical studies of these oleamides gave results that could be correlated with those previously obtained for a similar structure.

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A REVIEW OF MATHEMATICAL OPTIMIZATION APPLICATIONS OF DIET THEORY

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The problem of choosing the optimal diet for institutions has been studied since 1937 by Danzig. He introduced statistical elements in assessing the impact of nutrients used in food allocated to forces soldiers from CAF, and tried to determine the right level of sugar, calories and vitamins.

Later, Jack Laderman from the National Bureau of Standards has continued to develop a statistical model to determine the optimal necessary links between the ingredients and the amount of food needed to be consumed.

The present study includes applied mathematics selected for dietary theories (linear programming, multiobjective programming, Monte Carlo method) using both classical resolution (simplex method) and software developed for this problem.

In this study, the methods are analyzed and the best software (Win QSB, Exxel or QM) is selected.

A REVIEW OF MATHEMATICAL OPTIMIZATION APPLICATIONS OF TRANSPORT THEORY

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Optimizing transport of food interests both the scientific world and the major manufacturers.

Therefore, the development of several mathematical methods (linear programming, dynamic programming, inventory theory, the theory of the road map, Monte Carlo theory) led to achieving optimal transport routes.

Since 1859 (Carey) models and routes were created to optimize the transportation.

The present study brings into the spotlight the most advanced methods of developing optimal transport routes, analyzed both theoretically but also in terms of software developed for this area.

STUDY OF THE EFFICIENCY OF PLATE HEAT EXCHANGERS IN MILK INDUSTRY

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The plate heat exchangers are usually used in the food industry and they transfer heat from an ambient to another one. The applications of plate heat exchangers in food industry vary over a wide range. The aim of this study was to develop a computational dynamic fluid (CFD) model in order to evaluate the behavior of flat and corrugated plate heat exchanger when used in milk pasteurization process. These types of heat exchangers used in the milk pasteurization process flow are made from conventional stainless steel.

It was found efficiency of the plate corrugate heat exchangers is higher than of flat plate. This conclusion is also supported by thermodynamic optimization results taking into account heat transfer versus pressure drop.

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