ABSTRACTS

FRI- ONLINE-KS(R)-01

COMPUTER VISION APPLICATION IN THE QUALITY EVALUATION OF CEREAL-BASED PRODUCTS

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Abstract: *Humans do the visual inspection and quality control of many bakery products relying on the use of the sense of sight. Human inspection is a slow process, has poor repeatability and result varies from person to person. Computer vision system (CVS) is becoming one of the most important non-destructive, rapid, economic, consistent and objective inspection and evaluation technique in the food industry.*

This inspection approach is based on image analysis and processing of many products from food industry for objective evaluation of quality parameters of the product. Its speed and accuracy satisfy ever-increasing production and quality requirements, and offers the potential to automate manual grading practices thus standardizing techniques and eliminating tedious human inspection tasks.

This paper is dealing with CVS application for quality inspection of the cereal-based product. This method is applied for the inspection and grading of cereal-based products based on shape, size, colour and internal structure. According to the obtained results, CVS can been successfully adopted for the quality analysis of many cereal-based products such as bread, cookies, crackers, pizzas, etc. Furthermore, the CVS method proved to be successful for examination of the wheat grain quality.

Keywords: *Non-Destructive Methods, Image Analysis, Computer Vision, Cereal-based Products, Physical Properties*

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FRI- ONLINE-KS(R)-02

FTIR MICRO-SPECTROSCOPY FOR STUDY INHOMOGENIOUS PHASE COMPOSITION AND STRUCTURE OF BIOLOGICAL MINERALIZATIONS

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Abstract: *Infrared micro-spectroscopy is a powerful tool, sensitive to chemical and structural inhomogeneity, phase impurities, isomorphic substitution, degree of structural disorder, crystal size and orientation. This method and various techniques for its application are very suitable for the study of biologically formed mineralized hard tissues which have a complex structure and specific crystal-chemical properties. The most highly mineralized tissues in vertebrates are the teeth, which are composed mainly of non-stoichiometric hydroxylapatite* $Ca_5(PO_4)_3(OH)_2$*. This paper presents the spectral differences between healthy tooth enamel and dentine, which are basic in the study of changes resulting from pathology, dental treatment or external factors. Examples of pathological mineralizations such as urinary stones with various composition, identified by infrared spectra are presented. Also, the differences in the use of reflection and ATR infrared microspectroscopy are considered. This paper summarizes the advantages of the method and focuses on the information that can be extracted not only for the inhomogeneities in phase composition, but also for the structural characteristics of the most common mineralizations of biological origin.*

Keywords: *Infrared microscopy, biological mineralization, inhomogeneity, phase composition, structure*

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FRI-ONLINE-KS(R)-03

AN INTEGRATED APPROACH FOR WALNUTS INDUSTRIAL PROCESSING

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Abstract: *Walnut is a crop of a high economic interest for the food industry. Their major constituents are tryglicerides, in which monounsaturated (oleic acid mainly) and polyunsaturated fatty acids (linoleic and α – linolenic acids) are present in high amounts. The content of other bioactive components, such as proteins, tocopherols and phytosterols, has been also documented. Walnut kernel is appreciated as specialty nut also because of its characteristic flavor, aroma and health benefits. Walnut kernels are consumed fresh or toasted, alone or in other edible products. A major goal in walnut industry is to develop an integrated approach for walnuts processing to obtain large range of high quality food products. In this contribution, the development and characterisation of vegetable milk, oil and bioactive compounds derived from walnuts and their by-products is studied. Potentially walnuts were used to obtain these foods, not only able to exert health benefits, but also as an alternative to other food products. Processing steps and conditions to ensure chemical composition, quality properties, structure and rheological behavior of walnut based food products were analysed. These studies showed high potential and positive view on walnut industrial processing, in agreement with the current demand of healthy products. These results offer new interesting expectations to continue with this research line and demand the application of advanced technologies to provide better quality of the walnut products.*

Keywords: *Walnut, processing, high quality food*

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FRI- ONLINE-1-CT(R)-01

APPLICATION OF CHEMOMETRIC METHODS COUPLED WITH INFRARED SPECTROSCOPY FOR DETERMINATION OF ETHANOL IN PRESENCE OF METHANOL IN AQUEOUS SOLUTIONS

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Abstract: *A fast and cost-effective method, based on Fourier Transformed mid-Infrared Spectroscopy measurement coupled with chemometric method was developed for determination of ethanol in aqueous solutions at room temperature and presence of methanol. In order to facilitate the calibration process, and to minimaze the effects of peaks' overlapping, an appropriate preprocessing of the IR signals was performed. The calibration was performed using 43 samples, with accuracy enough high, so that this method can be used in routine determinations of ethanol. The model was also tested on a separate set of other 9 validation samples, where it showed great performance with R2 of prediction >0.99. Consequently, the procedure can be used as a fast and reliable determination of ethanol in aqueous solutions containing methanol as a second alchohol. The method can therefore find application in different areas of the chemical and food industry, avoiding use of chemicals, consumatives or expensive equipment as HPLC. In fact, this approcach could be used in other applications where distinguishable signals in FTIR exist, as for example quality control in production of fuels, essential oils, biodiesel, drugs etc.*

Keywords: Partial least squares, chemometric, FTIR, calibration, ethanol, methanol

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FRI- ONLINE-1-CT(R)-02

ELUCIDATION OF THE BINDING AFFINITY OF 2-CARBAMIDO-1,3-INDANDIONE TO NUCLEIC ACIDS

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Abstract: *Indan-1,3-dione is a biologically inactive compound, but its 2-substituted derivatives are biologically active and have aroused serious interest in the recent decades. They are used in medicine and biology . Studies on their biological activity show the presence of anticoagulant, anti-inflammatory, antibacterial, protein-binding, antineoplastic and neuroprotective action. The photophysical properties of CAID and its possible application as a sunscreen and biomarker have recently been investigated. It shows very good photostability and absorbs light in part of the visible region (400–450 nm), UVA (320–400 nm), UVB (290–320 nm) and UVC (200–290 nm). CAID is suitable as a biomarker in the study of biologically important molecules because it absorbs and fluoresces in a very wide spectral range and has a high quantum yield. Fluorescent and computational methods were used to elucidate the binding expedient of 2-carbamido-1,3-indandione (CAID) tautomers, 2-(hydroxylaminomethylidene)-indan-1,3-dione and 2-carboamide-1-hydroxy-3-oxo-indane, to DNA and RNA nucleotides. The dependence of the fluorescence emission of CAID loaded nucleic acids sequences to 2-carbamido-1,3-indandione concentration, temperature and time variation was investigated. It was found from the fluorescence data that the subject compound binds to nucleic acids but does not intercalate. Quantum-chemical calculations were performed to clarify the binding expedient of the complexes between nucleotides and CAID. According to the experimental and theoretical results, the binding may be through hydrogen bonds. Because of the binding affinity of CAID to nucleic acids we decided to perform a survey on the cytotoxic, antitumor and antiproliferative effects of CAID on three types of tumor cell lines - hepatic carcinoma, cervical carcinoma and rhabdomyosarcoma as well as one untransformed line - lung fibroblast cells. CAID demonstrated the most significant antiproliferative activity against the rhabdomyosarcoma cell line in a concentration of 0.0001 mg/mL equal to the maximal nontoxic concentration. Because of the binding affinity to nucleic acids and the lack of cytotoxic effect on non-tumor cell lines, we can suggest that the subject compound could be suitable to be used as a novel type of fluorescent biomarker.*

Keywords: *2-carbamido-1,3-indandione, fluorescent biomarker, cytotoxicity*

FRI- ONLINE-1-CT(R)-03

PHOSPHORUS RECOVERY FROM SWINE SLURRY BY ACIDIFYING ULTRAFILTRATION AND STRUVITE CRYSTALLISATION

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Abstract: *Recovering nutrinets form waste is an alternative to the continues phosphorus mining and fertilizers productin. Domestic wastewater and waste streams from livestock are among the most promising sources of recycled phosphorus with potential application in the agriculturing. The paper reviews a method of phosphorus recovery from swine slurry using stages of acidifying, ultrafiltration and cryzstalisation with an aim to extract phosphorus, purifying the fluid and sediment struvite crystals. The purpose was to examine the application of swine slurry, to establish pH-optimum for acidifying and crystalisation. Testings of orto-phoshorus, ammonium and magnesium were carried out on every step of the examination, also they were accompanied with supporting tests which indicated the decreasing of organic matter.*

Based on the results obtained, a procedure for acidic mobilization of the phosphates was developed as an initial step which significantly increased efficiency and recovery rate (up to 65%). Thereby the precipitation of struvite from wastewater and manure could be a step toward the development of hybrid technologies for simultaneously wastewater treatment and resource recovery which will contribute to the transformation of the economy from linear to circular approach.

Keywords: *phosphorus, swine slurry, manure, ultrafiltration, struvite*

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FRI- ONLINE-1-CT(R)-04

COMPARATIVE ANALYSIS OF BIOGAS PRODUCTION TECHNOLOGIES USING SUITABLE RAW MATERIALS

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Abstract: *The continuous increase in greenhouse gas emissions due to the rapid development of technical progress, as well as the growing needs for electricity require serious attention to the so-called "green energy" in order to meet permanently the needs of modern human society along with reducing emissions from greenhouse gases. Due to the natural putrefactive processes processes in the terrestrial flora and fauna, even without human intervention, significant amounts of gases (mainly methane) are generated, which can be used as green energy. Otherwise, they act as pollutants with the most serious greenhouse effect.*

The present paper focuses on the research of biogas production technologies, evaluation of raw materials and products, careful study and evaluation of all possible flows of raw materials and products, as well as environmental impact assessment as result of this activity.

Keywords: *Biogas, Anaerobic digestion, Bioenergy, Life-cycle assessment, Sewage sludge*

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FRI- ONLINE-1-CT(R)-05

TAUTOMERIC CONVERSION OF 2-CARBAMIDO-1,3-INDANDIONE UNDER INFLUENCE OF EXTERNAL ELECTRIC FIELD OR UV LIGHT

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Abstract: *2-Carbamido-1,3-indandione (CAID), also known as 1,3-dioxo-2-indanecarboxamide, exists in the solid state as yellow-orange needles which sinter from 180^{0}C to 220^{0}C. CAID exists in solution in two tautomeric forms, 2-(hydroxyl-aminomethylidene)-indan-1,3-dione (**A**) and 2-carboamide-1-hydroxy-3-oxo-indan (**B**). The structures of both tautomers as well as the transition state for intramolecular proton transfer are located at MP2/6-31+G(d) level of theory for each magnitude and for opposite directions of the applied electric field. According to our SCS-MP2/6-31+G(d) field-free calculations the tautomer **A** prevail (59.3 %) while variation of the electric field strength along the direction from the indandione moiety to the carbamido fragment leads to stabilize of tautomer **B**, and at 25.7x10^8 V.m^{-1} electric field strength, the ratio drastically changed: 98.05 % **B** and 1.95 % **A**.*

The tautomerization of CAID, A ↔ B, could occur thermally through a low energy barrier, 3.4 kcal mol^{-1}, or photophysically by internal conversion through a conical intersection S_0/S_1 and along the $^1\pi\pi^*$ excited-state reaction paths. The optic transitions $^1\pi\pi^* \rightarrow S_0$ are competitive reactions to the photophysical process. These optic transitions lead to the appearance of fluorescence bands, which should overlapped for the two tautomers, i.e. the two tautomers cannot distinguished by their fluorescent spectra only.

Keywords: *2-Carbamido-1,3-indandione, tautomerism, conical intersection, electric field, ab initio*

FRI- ONLINE-1-CT(R)-06

ASSESSMENT OF THE PERSONALITY OF PEOPLE, WORKING IN TECHNOLOGICAL SYSTEMS, WITH EYSENCK PERSONALITY QUESTIONNAIRE

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Abstract: *The study of personality characteristics with the Eysenck personality test aims to assess the intelligence, social attitudes and overall image of a person working in a risky technological environment. The personality questionnaire will provide results on three main indicators of personality: "Lie", or how strong the desire of the person to "fit" into the environment, based on imaginary rather than real qualities; "Extroversion", or the degree of open expression of feelings; and "Sensitivity," or "Neuroticism," which determine an individual's emotional resilience. The individuals selected for evaluation work in a complex technological environment in which emotional stability and the ability to make adequate and objective decisions is of great importance. Very often, working in such an environment requires the employee to have authority and gain the trust of his colleagues, being an active part of the work society, in which it may be necessary to make difficult decisions to prevent risk situations, minimize and manage risk.*

Keywords: *Hans Eysenck, Professional psychology, Technological risk assessment*

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FRI- ONLINE-1-BFT(R)-01

KINETIC ANALYSIS OF BIMOLECULAR COMPLEMENTATION "VIRUS - HOST-CELL" BY SURFACE PLASMON RESONANS (SPR) METHOD

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Abstract: *Since viruses are obligate intracellular parasites, they may exist and reproduce only in living host cell. In this bio-complex, the cell, in the role of host, provides its own structures and biosynthetic activity, but in accordance with the viral genetic program and with the direct participation of viral regulatory structures. Herpes simplex virus infections (HSV) are ubiquitous and widespread in the human population and represent a suitable model for study of virus-cell interactions. The aim of the present study is to detect and to evaluate the kinetics of a bimolecular "cell-host – herpes simplex virus" interaction in a condition of one-step virus growth infectious process using the surface plasmon resonance (SPR) method at different multiplicity of infection (MOI) and time of exposure. The obtained results are compare with other widely applicable methods such as microscopic observation of structural changes of infected cells and assay for detection of cell proliferation and survival. Human embryonal lung cells (Lep cell line) cultured at a density 3 x 10^3 cells/ml, post infected with HSV type 1 (HSV-1) with different MOI (0.01 and 0.1) were used. The cell survival and the structural-morphological changes associated with the different phases of the progression of the infectious process were evaluated by several methods: microscopic observation of changes in the morphology of the cell monolayer, MTT-assay and SPR technique. Cell survival and cytopathic changes are recorded at different intervals, which coincide with the different stages of the replication cycle of HSV-1 (3h, 6h, 8h, 12h, 16h, 24h and 48h). The obtained results from the SPR-method indicate accurate determination of the latent period at different MOI. The SPR method allows differentiation of the eclipse period from the latent phase, as well as determination of its duration at different MOI. The beginning of the latent and exponential phase (released virus) determined by the SPR method coincide with the structural-morphology changes registered by microscopic observation of the cell monolayer and with the reported survival rate by the MTT-assay. From the obtained results, can be concluded that the SPR method is promising and could be used to assess the bimolecular interaction "host-virus" in vitro and for the laboratory diagnostic of many infectious.*

Keywords: *SPR method, multiplicity of infection (MOI), HSV-1, MTT-assay*

FRI- ONLINE-1-BFT(R)-02

ANTIVIRAL EFFECT OF *GRAPTOPETALUM PARAGUAYENSE* E. WALTHER LEAF EXTRACT AND ITS PHENOL ACIDS FRACTION AGAINST HUMAN CORONAVIRUS 229E (HCOV-229E) *IN VITRO*

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Abstract: *It is known that some members of the Crassulaceae family possess several bio-medical benefits. Graptopetalum paraguayense E. Walther (GP) is a herbal medicine, belonging to this family. However, there is limited information in the literature on the antiviral, anti-oxidant and anti-inflammatory activities of this succulent plant. Of interest of investigation is also a plant hydroxybenzoic acids fraction, such as gallic acid, trans-ferulic acid, syringic acid, and others.*

The objective of our work was to evaluate, using colorimetric assay, the in vitro anti-human alpha coronavirus activities of Graptopetalum paraguayense E. Walther and its phenolic acids fraction in cell culture.

To evaluate the main organic groups, which had the aqueous leaf extract of the tested ethno plant was performed GC/MS analysis. To determine the capacity of the extract and its phenolic acids fraction (PAF) to inhibit the replication activity of human coronavirus strain 229E (HCoV-229E), as well as to evaluate the reduction of viability of infected or uninfected cells was used the MTT colorimetric assay. The results were expressed as maximal nontoxic concentration (MNC), 50% cytotoxicity (CC50) for MTT assay and 50% inhibitory concentration of the viral effect (IC50) for cytopathic effect (CPE) and MTT assay. The GP extract and PAF have not cytotoxic effect on human lung embryonal fibroblasts (Lep). The GP extract effectively inhibited HCoV-229E replication in dose-dependent manner. Furthermore, the GP extract was more effective inhibitor of HSV-1 replication in cultured cells (62%), whereas their PAF possessed lower effectivity (41%). The IC50 values range from 22.4 ± 0.2 to 88.2 ± 7.7μg/mL. According to results obtained, this plant extract protect cells against HCoV-229E infection, but the mechanism of their antiviral action and the active substancesare not yet completely identified. Further studies are needed in order to verify which compounds could be responsible for this activity and how they exert their antiviral effects.

Keywords: *Graptopetalum paraguayense E. Walther, GC/MS, hydroxybenzoic acids coronavirus, cytotoxicity, in vitro*

Acknowledgements: *This work was supported by the Bulgarian National Science Fund under Grant DN19/16/2017.*

FRI- ONLINE-1-BFT(R)-03

EMERGING APPLICATIONS OF IONIZING RADIATION FOR PROCESSING OF MATERIALS IN BIOTECHNOLOGIES AND FOOD INDUSTRY

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Abstract: *Ionizing radiation interacts with the materials by modifying their molecular structure and chemical composition. These changes substantially affect basic functional and technological properties of the materials such as strength, elasticity, plasticity, hardness, thermal conductivity, phase transition temperatures, chemical resistance, etc. This provides a possibility for using ionizing radiation for developing of new innovative materials, modification of existing materials with the purpose of improving their characteristics and processing of waste materials. The paper presents an overview of emerging modern radiation-based methods for treating of materials used in biotechnologies, food processing industry and food packaging and assesses the possibilities and benefits these technologies provide.*

Keywords: *ionizing radiation, materials, processing, modification, food, biotechnologies, packaging, innovation*

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FRI- ONLINE-1-BFT(R)-04

GAS PERMEABILITY OF BREAD

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Abstract: *The article presents the results of research of the permeability crust and central layers of bread products by gas, produced and transported from the workpiece to the environment during the vacuum cooling.*

It is proposed a scheme of laboratory installation and experimental procedure to study the permeability of the layers of the bread. Investigated the impact of temperature and humidity of samples on the value of permeability. It is found values of gas permeability of bread crust in different zones of a surface of workpiece. It is proposed the methods for calculating surface areas for round and oval workpieces. It is found unit gas flow rates through the surface of products during vacuum cooling.

The results can be used to determine the modes in which the vacuum provided the integrity of workpiece.

Keywords: *Bread, Vacuum, Cooling, Gas permeability.*

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FRI- ONLINE-1-BFT(R)-05

FORMATION OF SUSPENSION STRUCTURE IN THE PROCESS OF GRINDING IN BEAD MILLS

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Abstract: *It has been investigated the rheological properties of the suspension of farmaceutical and cosmetics preparates during grinding at an experimental laboratory bead mill of periodic action. The rheological characteristics have been investigated on a rotary viscometer Reotest 2. As a result of the research, the flow curve of the suspension during grinding has been constructed and it has been found that within the investigated range the product does not change the character of flow regardless of measurement time and temperature. Analysis of the curve of the suspension during grinding revealed features which explain formation of the structure. The dependence of the effective viscosity on the shear rate during grinding of the suspension is polynomial and confirms the non-Newtonian character of the product and is defined as a linear plastic body. The investigated finished product has 6.5 time's higher viscosity in relation to pure castor oil, which is explained by the high dry matter content (40 %) and the increase in the newly formed area. The viscosity of the suspension varies depending on the temperature: cooled to 20 °C, the finished product has a viscosity of 22.5% higher than immediately after the grinding process with a temperature of 34 °C.*

Keywords: *grinding, suspension, shear stress, shear rate, effective viscosity.*

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FRI- ONLINE-1-BFT(R)-06

STUDYING AND IMPROVING THE CONTINUOUS PROCESS OF KNEADING YEAST DOUGH

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Abstract: *A study of the process of kneading wheat yeast dough with cam working was conducted. The aim is to determine the rational configuration of structural elements for continuous kneading of dough at different levels of frequency of the working elements rotation and the distance between them.*

The kneading of wheat yeast dough by cam working elements is investigated. Mathematical modeling was performed using the Flow Vision software package based on the simulation of three-dimensional motion of liquids and gases in technical structures, as well as for the visualization of flow curves by computer graphics. Physical modeling was performed via experimental setup with cam kneading elements.

As the rotational speed of the working elements increases from 20 to 100 rpm, the mixing speed increases from 0.1 to 0.6 m/s, the distance between the cams does not affect the mixing in the specified range. The maximum values of pressure reach 16560 Pa for the distance between the cam working elements 2 mm and a speed of 100 rpm, the minimum 555 Pa for the distance between the cam working elements 10 mm and a speed of 20 rpm. In the mixing chamber, the highest-pressure values are formed in the contact zone of the cam working elements with the wall of the mixing chamber and in the contact zone of the two cams. The dependence of the viscosity in the mixing chamber on the speed of rotation of the working element is of a power nature and with increasing speed from 20 to 100 rpm decreases from 1600 to 320 Pa·s. Parts of the mixing chamber in which viscosity values in the range from 320 to 960 Pa·s are achieved are considered to be the most effective during mixing. Reducing the viscosity of the dough involves reducing energy costs during kneading.

To increase the carrying capacity of the cam working elements, improve mixing and reduce heat consumption, it is rational to use cam working elements with a variable pitch and a variable position of the cams at α = 45° or a combined cam working element using a screw auger at the beginning of the working element.

Keywords: *Modeling, Mixing, Yeast Dough, Kneading, Cam.*

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FRI- ONLINE-1-BFT(R)-07

EFFECT OF PROCESSING WITH ALTERNATIVE NON-THERMAL TECHNOLOGIES AND EDIBLE PACKAGING ON FOOD SAFETY AND QUALITY

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Abstract: *New technologies for food processing and packaging are aimed at creating products for end customers with minimal loss of quality. In this regard, in the field of food science, processes are developed that spare raw materials and food products, with minimal impact on them and causing minor changes in their initial characteristics. They are considered non-traditional and alternative to the treatments used so far in mass food production. The effect of them is only now beginning to be studied in more depth. The results obtained so far show that they have a future.*

To ensure the safety of minimally processed raw materials and food products, as well as to preserve their properties for a longer period of time, a set of impacts is applied, which are known as technology with the application of more obstacles to spoilage reactions.

The article reviews literature sources that publish information on combined methods of food processing, for the packaging of which edible films or coatings are used. Results from the application of various barriers to specific food products are indicated. Based on the analysis, conclusions are made about the possibilities for practical implementation of the technology with obstacles in the food industry in combination with the use of edible films and coatings.

Keywords: *Edible Packaging, Edible Films, Edible Coatings, Non-thermal Processing,*

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SAT-ONLINE-P-2-CT(R)-01

PREDICTING MOLECULAR PROPERTIES AND BIOACTIVITY SCORE OF SIMILAR COMPOUNDS OF TAZAROTENE

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Abstract: *The purpose of present work was to define with a Tanimoto similarity metric of 0.8 similar compounds of tazarotene and to predict and analyze theirs molecular physicochemical properties and bioactivity score by the CompTox Chemistry Dashboard and Molinspiration software. The data analysis for the three similar compounds of tazarotene were found to have close molecular properties and structural features and their bioactivity score is active.*

Keywords: *tazarotene, similar compounds, predict, bioactivity score, molecular properties.*

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Molinspiration Chemoinformatic Software, URL: https://www.molinspiration.com/

SAT-ONLINE-P-2-CT(R)-02

QUANTUM-CHEMICAL AND DOCKING ANALYSIS ON THE BINDING POTENTIAL OF HYDROXYBENZOIC ACIDS FROM *GRAPTOPETALUM PARAGUAYENSE* E. WALTHER TO HSV THYMIDINE KINASE ACTIVE SITE

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Abstract: *Herpes simplex virus types 1 and 2 (HSV-1 and HSV-2) are members of the Herpesviridae family and are among the most common human pathogens, infecting about 90% of the world population. HSV thymidine kinase (TK) catalyzes the transfer of the gamma-phosphate group of ATP to thymidine to generate dTMP in the salvage pathway of pyrimidine synthesis. The dTMP serves as a substrate for DNA polymerase during viral DNA replication. TK allows the virus to be reactivated and to grow in non-proliferative cells lacking a high concentration of phosphorylated nucleic acid precursors. Thus, TKs are the main targets in anti-herpes virus treatments and potential therapeutic targets in antitumor gene therapy strategies. Recently we found that the total methanol extract from the succulent plant Graptopetalum paraguayense E. Walther (GP) demonstrates/has a significant inhibitory effect on HSV-1 as well as the GP phenolic fraction.*

Since TK appears to be a key feature in the replication of large DNA viruses such as HSV, we present theoretical investigations on the binding expedient of phenolic acids from this fraction to viral TK amino acids. Twelve different hydroxybenzoic acids such as gallic acid, trans-ferulic acid, syringic acid, and others were found by GS/MS analyses.

MOE 2016 software package was used to dock selected structures in the active site defined in published XRD (X-ray diffraction) structures of the Herpes Simplex Virus 1 thymidine kinase. The structure was protonated according to implemented Protonate3D algorithm and was scored according to implemented GBVI/WSA dG scoring function. The interaction energies of ligands (phenolic acids) in the pockets based on the GBVI/WSA dG scoring function were sorted and four best ligands according to ligand-pocket interactions were selected: trans-ferulic, gallic, syringic and gentisic acids have optimal interactions with the receptor.

From the results based on the molecular docking methods, different types of hydrogen-bonded complexes of hydroxybenzoic acids with amino acids, protonated amines, mineral acids and water molecules were modelled. The data received from our quantum-chemical calculations suggest that all twelve phenolic acids could form stable complexes with amino acids from the TK active site. The complexes formed are stable and trans-ferulic and gallic acids demonstrate great binding affinity to the active site of TK where they can exhibit their inhibitory properties. The calculations were performed at B3LYP/6-31+G(d,p) level of theory using GAUSSIAN 09 software package.

Keywords: *Graptopetalum paraguayense E. Walther, thymidine kinase, Herpes Simplex virus, docking, quantum-chemical calculations, hydrogen-bonding.*

Acknowledgements: *This work was supported by the Bulgarian National Science Fund under Grant DN19/16/2017.*

SAT-ONLINE-P-2-CT(R)-03

GREENHOUSE GAS REDUCTIONS THROUGH OPTIMAL BIODIESEL SUPPLY CHAIN

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Abstract: *In the last few decades, attention has been focused on the world scientific community for prioritizing global closure, depletion of the ozone layer in the atmosphere and the danger to nature in general. A number of factors are analyzed, the influence on these processes is shown, as well as optimal opportunities for achieving sustainable development. One of these factors is emissions from the transport sector. The purpose of this article is presented on biodiesel as an alternative to conventional diesel fuel, contributing to the reduction of greenhouse gas emissions, provided for the entire life cycle of the fuel. The article presents a mathematical model of a Supply Chain for the production and distribution of biodiesel with the help of one that determines optimal values with minimal environmental pollution. A case for the Republic of Bulgaria is being considered.*

Keywords: Biodiesel, Biodiesel blends, Emission, Supply Chain.

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SAT-ONLINE-P-2-CT(R)-04

INVESTIGATION OF ELECTRICAL CHARACTERISTICS OF BARIUM TITANATE ($BATIO_3$)

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Abstract: *A technology for synthesis of barium titanate ceramics with high dielectric constant is proposed. In present work a sol-gel method was used for $BaTiO_3$ synthesis. Different mixtures have been studied and the technological regimes for obtaining a quality ceramic structure with high dielectric constant have been optimized. This ceramics could find application in the development of dielectrics for supercapacitors.*

Keywords: *Barium titanate, dielectric, supercapacitors*

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SAT-ONLINE-P-2-CT(R)-05

MODIFICATION OF ULTRAFILTRATION POLYACRYLONITRILE MEMBRANES WITH NANOCLAY PARTICLES

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Abstract: *Polyacrylonitrile/nanoclay composite membranes were prepared by phase inversion of 17wt.% solutions of polyacrylonitrile (PAN) with various amounts of Nanomer 1.28E in solvents dimethylsulfoxide (DMSO) and dimethylformamide (DMF). Changes in the characteristics of PAN membrane before and after heat treatment and in dependence of the amount of nanoclay particles were observed by atomic force microscopy (AFM) and studied by the rejection (R, %) and permeability (J, l/m^2.h) to albumin and hysteresises relative to water constructed at J=f(P) at P=0.1- 0.5 MPa. The results show that nanoclay particles have a modifying effect and importance for the operational stability and characteristics of the membrane structure most effective at 1.5 wt.% of Nanomer 1.28E. The corresponding membrane reaches a water permeability from 110 to 188 l /m^2.h, the selectivity from 30 to 70 % with a mean square roughness (Rmax) of the surface up to 58.4 nm.*

Keywords: *polyacrylonitrile , nanoparticles, nanocomposite, polymer membranes*

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SAT-ONLINE-P-2-CT(R)-06

CORDIERITE CERAMICS WITH IMPROVED PERFORMANCE PROPERTIES

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Abstract: *Cordierite ceramics have found wide application in various branches of science and technology. Its distinctive feature is a low coefficient of linear expansion. However, it is practically impossible to obtain ceramics with zero porosity. Therefore, the study investigated the possibility of obtaining cordierite ceramics with improved performance characteristics. As a result of the development of the initial chemical composition of the base composition, it was possible to obtain materials with the following properties: porosity 1,4%, density 2.07 g/cm^3, compressive strength 130 MPa, temperature coefficient of linear expansion 19,2·10^{-7} deg^{-1}.*

Keywords: *Cordierite, Thialite, Porosity, Compressive strength, Temperature coefficient of linear expansion*

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SAT-ONLINE-P-2-CT(R)-07

CHANCES OF UTILIZING OF SPENT CATALYSTS FROM PETROCHEMICAL INDUSTRY

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Abstract: *The article investigates the possibility of utilization of spent catalyst from petrochemical industry. These waste products in combination with natural raw materials could be materials for a development of wide variety of products and can be successfully implemented in to industrial production.*
Keywords: *Spent Catalyst, Petrochemical Industry, Waste, Ecology*

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SAT-ONLINE-P-2-CT(R)-08

STUDY OF THE COLOR PARAMETERS OF ZIRCON CERAMIC PIGMENTS SYNTHESIZED FROM PURE RAW MATERIALS

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Abstract: *Zirconium ceramic pigments with basic zircon phase - $ZrO_2.SiO_2$ were synthesized by solid phase sintering of pure oxides: ZrO_2, $SiO_2.nH_2O$, and the following elements were added as colorants: V, Fe, Cr, Co and Mn. NH_4Cl was used as a mineralizer. The pigments were synthesized at three final firing temperatures: 1000, 1100 and 1200 ° C. The color characteristics of the synthesized zirconium ceramic pigments were determined using a color measurement system - CIELab.*

Key words: *zircon pigments, solid-state sintering, CIELab color measurement*

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SAT-ONLINE-P-2-CT(R)-09

CORROSION INHIBITION OF LOW-CARBON STEEL IN A 0.1 M H_2SO_4 MEDIUM

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Abstract: *In the present work, preliminary studies on the corrosion of low carbon steel in sulfuric acid medium with the addition of the organic substance 6-(10H-phenothiazin-10-yl)-1H,3H-benzo[de]isochromene-1,3-dione were performed. Its introduction into the corrosive medium (0.1M H_2SO_4) was carried out by its solution in ethanol. The gravimetric method was applied to determine the characteristics of the corrosion process. The corrosion rate, the degree of protection and the inhibition action coefficient were estimated by varying the concentration* $\left(5\times10^{-7}-5\times10^{-5}\right) mol\,dm^{-3}$ *of the inhibitor substance.*

The obtained results clearly show that this compound has the potential to successfully be employed as an effective corrosion inhibitor of low carbon steel in sulfuric acid media. However, due to its low solubility in ethanol, experiments have been performed to find other suitable polar solvents to enable the increase of its concentration in the corrosive environment.

Keywords: low-carbon steel, corrosion, inhibitors, acidic media, *6-(10H-phenothiazin-10-yl)-1H,3H-benzo[de]isochromene-1,3-dione*

Acknowledgement: The authors acknowledge the support of the Science Fund of the University of Ruse, Bulgaria (project 2020/BRz-01).

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SAT-ONLINE-P-2-CT(R)-10

FEATURES OF THERMAL DESTRUCTION OF COMPOSITIONS OF SPODUMENE-EUCRYPTITE COMPOSITION OBTAINED BY SOL-GEL TECHNOLOGY

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Abstract: *The article is devoted to the study of glass-crystalline heat-resistant materials of the oxide system Li_2O-Al_2O_3-SiO_2. These materials were obtained by the sol-gel method, which is an alternative to traditional methods of obtaining structural materials using ceramic and glass technology. In the course of research, strict parameters for obtaining these materials with a high degree of homogeneity of their structure have been worked out. However, it has been established that the stability of materials significantly depends on the conditions for their further heat treatment: despite the expected low-temperature decomposition of some components of the composition, the temperature of the irreversible transition of the material to a stable state shifts to the region of 700-800 ° C. This aspect is very important for long-term storage of the intermediate product.*

Keywords: *Sol-gel method, Heat-resistant glass ceramics, Spodumene, Eucryptite, Calcination*

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SAT-ONLINE-P-2-BFT(R)-01

STARCH SYRUPS AS SUBSTITUTES FOR SUGAR AND MILK POWDER IN ICE CREAM

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Abstract: *The article considers the existing and promising ways to use starch syrup in milk-based ice cream recipes. The influence of substitution of sugar on dry skimmed milk starch syrup and starch on the characteristics of mixtures for the production of ice cream of classical types has been investigated. To study the possibility of simultaneous replacement of sugar and dry skim milk residue with starch syrup in milk-based ice cream, the degree of substitution of the milk component up to 30% is used, which will ensure its minimum possible content in the product (at least 7%). Simultaneous replacement of milk powder and sugar on the composition of starch syrup with different carbohydrate composition has been carried out. The article describes the results of analytical and experimental research methods: rheological characteristics and cryoscopic temperature of mixtures, organoleptic characteristics of ice cream, whipped cream, resistance to melting. As a result of the conducted researches the multifunctional technological properties of starch syrup with low and high degree of saccharification in the composition of mixtures for ice cream production as sweeteners, cryoprotectants, thickeners and structure stabilizers has been revealed. Studies confirm the feasibility of using composite mixtures of low-sugar and high-sugar starch syrup as substitutes for sugar and milk powder in ice cream. On the basis of research, ice cream recipes with improved characteristics and reduced cost have been developed.*

Keywords: *sugar substitutes, ice cream, starch syrup, sweeteners*

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SAT-ONLINE-P-2-BFT(R)-02

MODELLING OF PROCESS OF PRESSING THE DOUGH IN MATRIX WITH SCREW INSERTS

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Abstract: *It is proposed to install special screw-shaped inserts in the matrix for the production of pasta. The inserts has has injection-type screws shape. This allows to regulate the process of pressing the dough, pre-compacting the dough, plasticizing it and simultaneously heating it.*

A smooth transition of the dough in the forming holes is ensured, the hydraulic resistance of the forming channels is reduced, the quality of pasta improves, the productivity of the press increases and the durability of the matrix operation is increased.

A mathematical model of a pumping-type auger has been built, which makes it possible to obtain the same dough compaction coefficient for all screw channel inserts. The mathematical model of the screw sweep more accurately takes into account the shape of the helical groove in the normal section –a shape close to a trapezoid, and not to a parabolic segment.

The use of special inserts in the matrix improves the quality of semi-finished products, increases the productivity of the screw press by 20%, and reduces the specific energy consumption.

Keywords: *pasta, dough, matrix, auger, seal.*

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SAT-ONLINE-P-2-BFT(R)-03

REASONING OF THE SELECTION OF TECHNOLOGICAL PARAMETERS FOR THE EXTRACTION OF SUMAC

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Abstract: *In order to intensify the extraction process, the possibility of using a rotary-pulse apparatus was investigated. The use of rotary-pulse extractors makes it possible to intensify the process of eliciting extractive substances of plant raw materials in comparison with traditional methods, to improve the microbiological parameters of the obtained extracts due to the tightness of the circuit and to ensure the energy efficiency of the process.*

It was found that with increasing temperature, the mass fraction of extractives increased, while the duration of the process at the selected temperature was of great importance. The duration of the extraction at a temperature of 20 ° C for 10 min, gave the same yield of extractives as heating the system "raw materials/solvents" to a temperature of 80 °C without endurance.

To compare the results of experimental data determined by different methods, the coefficient of variation was calculated. That is, the use of a rotary-impulse apparatus makes it possible to increase the yield of extractives by an average of 24.5% in comparison with classical maceration.

Keywords: *extraction, sumac, extractives, temperature.*

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SAT-ONLINE-P-2-BFT(R)-04

EVALUATION OF ANTIOXIDANT ACTIVITY OF HYDRAZONE

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Abstract: *Antioxidants are molecules that can prevent or slow damage to cells caused by free radicals. It is therefore important to determine the content and effectiveness of antioxidants in various chemical compounds and foods. This necessitates the development of a rapid method for determining the potential antioxidant effect. In the present study, we investigate the antioxidant potential of newly synthesized hydrazone of the antineoplastic drug bexarotene. The analyzes used (ABTS • + and DPPH) are widely used methods for assessing the antioxidant capacity of natural products. Both approaches are spectrophotometric techniques based on the quenching of stable color radicals. The DPPH method allows to determine the antioxidant activity by using a stable free radical - 1,1-diphenyl-2-picrylhydrazyl (DPPH; C18H12N5O6, M.m = 394.33). The study is based on measuring the suppression capacity of antioxidants to it. The antioxidant activity of the newly synthesized compound was also determined by ABTS [2,2'-azinobis (3-ethylbenzothiazoline-6-sulfonic acid)] cation radical decolorization method.*

Keywords: *Antioxidant activity, hydrazine, antineoplastic drug, bexarotene*

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SAT-ONLINE-P-2-BFT(R)-05

DEVELOPMENT OF COMPOSITE SAUCES FOR PASTEURIZED PRODUCTS

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Abstract: *The analysis of the market and trends in the sauce segment in Ukraine and around the world shows the orientation of consumers to healthy eating and the desire to consume environmentally friendly products. There is an active update of the range of sauces, because today the bulk of sauces produced by industry, falls on the segment of mayonnaise.*

Fruit-based emulsion sauce formulations have been developed. The possibility of regulating the emulsifying ability and stability of emulsions using different types of dispersion was studied (1). The pH value for plum-based sauces varies depending on the recipe 3.2-3.5, after heat treatment, at a temperature of 85°C the values do not change (2, 3).

For tomato-based sauces, the pH value is 4.6-4.9, after heating it decreases slightly.

Stability of technological indicators of sauces at heating allows to recommend them for production of pasteurized products, including pasteurized sausages and canned meat ( ).

Keywords: *sauce, pasteurization, emulsion*

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SAT-ONLINE-P-2-BFT(R)-06

BASIC PROVISIONS AND RESEARCH OF CONTINUOUS DOUGH KNEADING

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Abstract: *The development of a continuous-action dough-mixing machine is accompanied by the choice of a rational configuration of the working element. Rationalization is realized by analyzing the various configurations of the working element and its effect on the kneading process. Imitation modeling aims to calculate the values of certain characteristics of a process that develop over time, by reproducing the flow of this process on a computer via its mathematical model.*

During projecting of the process of dough mixing, there is a range of issues related to the type of working elements is supposed to be chosen. On the basis of theoretical searches and obtained experimental results, after comparative analysis of working elements, it was decided to simulate the process of kneading yeast wheat dough using cam working elements.

Obtaining information about the process of mixing at any point in the mixing tank using simulation modeling and the results of a physical experiment allow to project an effective working element in a high-tech continuous mixing machine.

Dough kneading is a complex process that involves creating a homogeneous capillary-porous mass of flour, water, yeast, salt, and other components. The formation of dough during kneading occurs as a result of a number of processes, of which the most important are: physico-mechanical, colloidal and biochemical processes. All these processes occur simultaneously, mutually affecting each other and depend on the duration of kneading, temperature and the amount and quality of raw materials used during kneading the dough.

Keywords: *Yeast Dough, Provisions, Continuous, Kneading.*

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SAT-ONLINE-P-2-BFT(R)-07

SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL STUDIES OF 6 – PHENOTHIAZINIL – 1,8 – NAFTHOYLENE – 1,2 – BENZIMIDAZOLE – 1 - OH

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Abstract: *The subject matter of this article is the synthesis of isomeric luminescent compounds with orange-red color, containing a phenylthiazine ring and a 1,8 - naphthoylene - 1,2 - benzimidazole group. The IR-spectra of the individual isomers formed in the process of synthesis, their separation and antimicrobial activity were studied.*

Keywords: *Phenothiazin, Synthesis, Isomers, Antimicrobial activity*

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SAT-ONLINE-P-2-BFT(R)-08

SIMULATION OF HIGH PRESSURE MEAT PATE PROCESSING

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Abstract: *For meat pies, it is common to use mathematical models to use regression analysis. Each time there is a change in experimental data, a new mathematical model is built, which changes the number of important independent factors and the values of their degree. Therefore, the use of regression equations in the theory of modeling the processes of microbiological synthesis does not allow to obtain the required accuracy of the results and for this reason their use can not be considered satisfactory.*

It is presented a new method of constructing a basic mathematical model for different types of pate in the form of a differential equation. The positive thing is that the characteristics of the model retain their dimensions: the magnitude of the pressure (Pa), the duration of its action (second), the optimization parameter - the magnitude of biological pollution (CFU). It makes it possible to determine the effectiveness of inactivation of microorganisms at different hydrostatic pressures and the duration of its exposure by the magnitude of the initial biological contamination of the pate mass.

A method has been developed that makes it possible, depending on the specific conditions of the technological process, to refine the optimization parameter. To do this, the exponent is additionally introduced into the mathematical model. This method of refining the mathematical model is well known, but the conditions for finding its value and other characteristics of the model remain imperfect and problematic.

Keywords: *meat, pate, pressure, modeling.*

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SAT-ONLINE-P-2-BFT(R)-09

SCIENTIFIC SUBSTANTIATION OF THE PROCESS OF MANAGING CRITICAL MODES OF PNEUMATIC TRANSPORTATION FOR FOOD PRODUCTS

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Abstract: *The mathematical and physical models for critical modes of pneumatic conveying has been developed to ensure calculations and design of the main pneumatic product pipelines with a continuous mode of operation. The model takes into account the technological conditions of the gas suspension movement; the laws of motion of individual small-piece particles, taking into account their impact interaction and decompression, as well as real boundary conditions for the movement of a food product. The parameters of the zone of dynamic destruction of the layer of small-piece food product by the air shock wave were experimentally investigated and the comparison of the calculation results with the experiment was performed. The process of controlling the critical modes of pneumatic conveying based on proportional elements and feedback (current loop 4–20 mA) was theoretically described; investigation of the process of destruction of a cluster of products using an air wave and controlled decompression. An approach to modelling pneumatic conveying systems as a whole is proposed. The total pressure loss in the pneumatic conveying pipeline is investigated, it consists of: pressure losses arising from the movement of clean air; additional pressure losses arising from the movement of material; pressure losses to maintain the transported material in suspension in a vertical section; pressure loss for acceleration of transported particles when they are drawn into the transport pipeline; which are directly proportional to the volumetric mass of air, the speed of its movement and the weight concentration of the material in the mixture.*

Keywords: *pneumatic conveying, small-piece, model, modes, boundary conditions, control, layer.*

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SAT-ONLINE-P-2-BFT(R)-10

FUNCTIONAL CHARACTERISTICS OF FOOD OF ANIMAL ORIGIN

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Abstract: *Due to the growing concern of consumers about their own health, nutrition and food quality, in recent years the food industry has focused on the development of food products with functional characteristics (functional food) that have a special specific composition and nutritional quality. Functional foods in addition to traditional nutrients contain functional (bioactive) ingredients that positively affect health and reduce the risk of disease. Functional foods can be foods that naturally contain functional components, foods that are "enriched" with functional ingredients, or foods that remove certain ingredients, which reduces the risk of developing some diseases.*

The functional characteristics of food of animal origin (milk, meat, egg) are the result of the natural content of functional components, due to which they have an irreplaceable role in nutrition globally.Incorporating bioactive ingredients in the processing of milk and meat (probiotics, prebiotics, antioxidants) or the replacement of some components (saturated fats) with components that have proven positive effect, allows the creation of functional dairy and meat products with favorable health and physiological effect. Today, the production of functional food is steadily increasing, and new products are increasingly accepted by consumers.

The paper is a review of literary data on the functional characteristics of different foods of animal origin and its importance in the diet.

Keywords: *functional food, bioactive ingredients, food of animal origin*

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SAT-ONLINE-P-2-BFT(R)-11

STRUCTURAL AND PARAMETRIC SYNTHESIS OF KNEADING MACHINES

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Abstract: *It are offered methods of analysis and research of hydrodynamic processes in kneading machines. In modern conditions, a qualitative full-fledged study of complex hydrodynamic processes that occur during the movement of the working bodies of the mixing equipment is impossible without the use of computer technology. Methods and programs of three-dimensional simulation computer modeling make it possible to obtain quantitative and qualitative characteristics of kinematic and dynamic processes. With the accumulation of a sufficient amount of information, it is possible to synthesize the design of the kneading machine, which will include technical solutions that allow you to create the optimal industrial design for today.*

The analysis of constructions of kneading machines and a technique of research of their work gives the chance to define directions both improvement of work of existing, and to create new variants of a structure.

Keywords: *mixing, bread dough, efficiency, modeling.*

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SAT-ONLINE-P-2-BFT(R)-12

PRACTICAL ASPECTS OF MODELING HYDRODYNAMIC CHARACTERISTICS IN THE SYSTEM OF PIPELINE VALVES

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Abstract: *Proper operation of control valves allows you to maintain the parameters of technological processes and increase the effect of juice purification and sugar yield, reduce the sugar content in molasses, reduce fuel consumption and milk of lime. Search for rational parameters. The technology of the control valve selection is offered in the work, on the basis of the analysis of the static characteristic of the working object. It is shown that when choosing the standard size of the valve according to the equations of flow and throughput characteristics, the operation of the valve is considered separately from the operation of the control system of flowing of modern sugar production. The technology of the control valve selection is offered in the work, on the basis of the analysis of the static characteristic of the working object.*

Empirical methods have been used to calculate the cost characteristics for evaluating the operation of control valves and shut-off elements. Models of the object of regulation on the experimental stand are investigated. The study of the transient process when emptying the working chambers proved the following - the time of the transient process depends on the initial pressure in the chamber, the volume and type of muffler installed on the exhaust of the regulator (creates additional resistance to working air during discharge). At an initial pressure of 5 bar, for V = 4 l at step change of a control signal, time of transient process at use of the muffler on an exhaust to 1,8s is accurately fixed. When reproducing the operation of the regulator without a muffler - the transient time is twice less.

Keywords: *control valves, parameters, technological processes, sugar yield.*

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