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Abstracts

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ADVANCES IN BIOMASS AND BIOGAS ENERGY

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There is strong scientific evidence that the average temperature of the earth's surface is rising and this may be attribute to increased concentration of carbon dioxide (CO_2), and other greenhouse gases (GHGs) in the atmosphere as released by burning fossil fuels. One of the chief sources of greenhouse gases is burning of fossil fuels. Biogas from biomass appears to have potential as an alternative energy source, which is potentially rich in biomass resources. In the present study, current literature is reviewed regarding the ecological, social, cultural and economic impacts of biogas technology. In this communication an attempt has been made to give an overview of present and future use of biomass as an industrial feedstock for production of fuels, chemicals and other materials. However, to be truly competitive in an open market situation, higher value products are required. Results suggest that biogas technology must be encouraged, promoted, invested, implemented, and demonstrated, but especially in remote rural areas.

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SYNTHESIS AND EVALUATION OF ZNO NANOPARTICLES AND STUDYING ITS INFLUENCE ON THE ANTIMICROBIAL, ANTICORROSION AND MECHANICAL BEHAVIOUR OF POLYURETHANE COMPOSITE FOR SURFACE COATING

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Zinc oxide nanoparticles (ZnO NPs) were obtained by a direct precipitation method. The TEM photograph demonstrated that the synthesized ZnO NPs were of a pseudo-spherical shape and the average diameter of the particles is 20.0 nm. ZnO polyurethane nanocomposite (ZPN) coating films were fabricated by uniformly dispersing ZnO NPs in varying loading levels 0.1 to 2.0 wt. % in commercial two component polyurethane by ultrasonication. The antimicrobial activity of ZPN coating films was screened against Gram-negative and Gram-positive bacteria. Corrosion performance, physical and mechanical properties of ZPN coating films was evaluated. The resulting perfect dispersion of ZnO NPs in polyurethane coating was revealed by SEM. The results showed slowdown of the growth of organisms on the ZPN coating surface and also showed an improvement in the corrosion resistance, mechanical resistance at lower concentration, and this improvement increases with increase ZnO NPs wt.%.

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EFFECTS OF DIETARY SATURATED FAT ON SERUM CHOLESTEROL LEVELS

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It is well established that diet is the primary therapeutic approach for persons who are at increased risk of premature heart disease, as a result of having elevated serum cholesterol levels (more than 200 mg/dl). Many dietary recommendations have been published in the last five decades that have advised people to reduce their intake of total fat, saturated fat and cholesterol to improve their cholesterol level and decrease the risk of coronary heart disease (CHD). However, these recommendations have recently been challenged by claims that dietary fat, saturated fat and cholesterol do not affect serum cholesterol levels and the risk of CHD. Dietary cholesterol as a nutrient of concern has been dropped by the Dietary Guidelines Advisory Committee (DGAC) report (2015), so as to accord with evidence that there is no appreciable relationship between dietary cholesterol and serum cholesterol or clinical cardiovascular disease (CVD). Moreover, the DGAC placed no limit on total fat consumption. Although evidence for an association between saturated fat intake and CHD remains controversial, it is widely accepted that saturated fats can raise serum levels of total cholesterol (TC) which increase is reflected in the low-density lipoprotein (LDL) fraction. A meta-analysis (Siri-Tarino et al. 2010) of prospective cohort studies has indicated no association between saturated fat intake and CHD. While a randomized trial (Dreon et al. 1998) has found that intake of saturated fats decreases the small-dense LDL-cholesterol fraction but increases the large-buoyant LDL-cholesterol fraction. High levels of large-buoyant LDL fraction may be resistant to oxidation and anti-atherogenic and therefore protective against CHD, whereas the small-dense LDL fraction is more susceptible to oxidation, is pro-atherogenic. High levels of this LDL fraction are associated with greater CHD risk. Hence, consumption of saturated fat may alter the ratio of these fractions and be protective against CHD. In this paper I will review the major published effects of dietary fat, saturated fat and cholesterol on serum cholesterol levels and the increased risk of CHD.

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INORGANIC NANO FILLER IN POLYMER NANOCOMPOSITES AND ITS THERMAL BEHAVIOURS

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Thermal analysis is one of the oldest technique for the analysis of materials for the test of materials to be genuine or fake, on the basis of simple heat test. Due to enormous advances in material sciences and day by day new materials are added up to the life of human being. So the quality and perfection is highly in need with features such as low weight, high tensile strength, excellent physical and chemical properties. Therefore, thermal characterization is an ideal tool for the determination of these parameter as well as other transition and materials properties. In this presentation, various research work performed on polymer nanocomposites of nano particles filler such as Calcium, barium, zinc, tin, silver were highlighted taking matrix as polymer. Research work performed by various scientists in polymer nanocomposites for material development using thermal analysis tool will also be discussed. Its future aspect, behaviors of Tg and Td with the increase in nanoparticles loadings in polymer matrix will also be highlighted. Various analytical tool such as XRD, FTIR, SEM, EDS, and UV-Vis spectrum of polymeric films of nano composites will also be used for correlation and characterization of materials.

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PRACTICAL USE OF AMINO ACIDS IN ONCOLOGY: REPLACEMENT THERAPY AS A STRUCTURAL COMPONENT OF PROTEINS AND/OR FOR CORRECTION OF METABOLISM IN QUANTITIES COMPARATIVE WITH THEIR ENDOGENOUS CONCENTRATIONS

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The aim of our research is the formulation of methodology creation for practical application of the regulatory action of endogenous (physiological) concentrations of separate amino acids or their pathogenetically justified compositions. Changes in amino acid pool in liquids and their tissues fund of oncology patients specifically characterize development of cancer and largely induced by metabolic competition between the tumor and the tumor carrier. Correction of the intermediate metabolic changes in cancer can be reached by the use of certain amino acids or their combinations. Based on the positions of metabolomics, the free amino acid pool in biological fluids and tissues is regarded as a single information unit which is a kind of "a chemical projection" of the genome. The proteome realized through this approach not only develops ideas about the pool of amino acids as a dynamical system-generated supply of them from outside, but also due to endogenous synthesis, transport, degradation and excretion and allows the identification of "key points" in intermediate metabolic equilibrium shift that may reflect ratios at the individual levels of endogenous amino acids and related species (metabolically-related) compounds to achieve "metabolic comfort." On the basis of the experimental data, we suggest that the differences discovered in certain amino acids concentrations in fluids and tissues are the criteria in early diagnostics as in estimation of the efficacy of specific cancer treatment. Our clinical studies on biological fluids and tumours of more than 1400 patients with cancer depending on the location and stage of the process showed significant changes in physiological concentrations of amino acids which either directly or indirectly regulate processes of antitumor response, oncogenesis, immunogenesis and apoptosis were shown. The creation methodology of pathogenetic compositions of amino acids and their derivatives on the basis of their physiological concentration for practical application of their regulatory effects in oncology was discussed.

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COMPOSITION OF PARAFFIN INHIBITOR FOR OIL AND OIL PRODUCTS

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Kazakhstan is paraffin, i.e. contains a significant amount of alkanes of normal or lightly branched structure. The latter type is characterized by an increased pour point, which causes deterioration of the rheological properties (mobility, fluidity, etc.) of both the oil itself and its products. This fact has a negative impact on the process of oil extraction and transportation, and therefore is a subject for research in order to improve the technological effectiveness of the oil industry. Prevention of crystallization of paraffin is possible by heating the oil to 50-60 ° C, but this method sometimes leads to unnecessary costs and is not economically justified. Lowering the crystallization temperature can be achieved by mixing high-paraffin oil with low paraffin or solvents, which also leads to additional time and resources. Many compositions of popular solvents and additives were studied, as a result of which we came to the final choice of the necessary components for the development of this additive. Numerous organic solvents were used as the solvent, but for this type of additive, it did not show satisfactory results, which led to a study of the characteristics of the desired solvents with suitable properties. A new composition paraffin inhibitor consisting of synergistic compositions combined pour point depressant and paraffin inhibition action based on a polymeric component and a composition of surfactants is presented. The most effective way to improve the low-temperature properties of oils, fuels and oils is the use of paraffin deposition inhibitors. These are substances, due to the introduction of which, even in small doses (usually 0.05-0.10%), substantial prevention of the formation of paraffin and an improvement in fluidity at low temperatures are achieved. Initial components were polystyrene foam and chloroform. Polystyrene foam was dissolved in a solution of chloroform after filtration. As a result of the laboratory tests, significant results were obtained, but results differed with changing concentrations of components. After carrying out numerous tests with varying concentrations of components, data were obtained that allowed to determine those values at which we obtained the most optimal rational values. To improve the low-temperature and viscosity properties of oil and oil products, such as diesel fuel, we proposed to use the inhibitor-based polymer. It was established that the inhibitor additive is a 10% polymer solution in a chlorine derivative alkane. Introduction of an additive based on PSA-10 in the amount of 100-1500 ppm in hydrotreated diesel fuel and oil shows a significant results of freezing point (Table 1). When comparing the temperature of solidified diesel fuel with the Dodiflow product additive, it was found that the effect of the PSA-10 inhibitor-based additive is more effective than in the case of the product additive. The freezing point of diesel fuel with PSA-10 additive is –35 °C, whereas when using the Dodiflow additive is –34 °C.

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Figure-1: Initial components: a) polystyrene foam

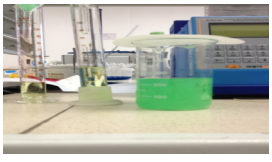

Figure-2: Initial components: b) mixture before filtration

Figure-2: Initial components: c) final inhibitor

Additive	Freezing point, ° C	
	Crude Oil	Diesel fuel
Without additive	-10	–20
Dodiflow	-21	–34
PSA-10	-23	-35

Table 1: Effect of additives to freezing point

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MOLECULE OF MILLENNIUM—TAURINE AND ITS ANALOGUES: A NEW CLASS OF THERAPEUTICS IN HUMAN WELFARE

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Chemicals are not single minded, in differ environment they me be friend or foe. Human body is reservoir of a large number of molecules with diverse nature of chemical identities influencing the mind and mood. Amino acids constitute a large portion with such agents. One of such agent is Taurine (2-Amino Ethane Sulfonic Acid). Its content is high in several human tissues like, heart, brain, liver, kidney and eye. Taurine is 0.1% of total body weight amounting 70 g in a normal human of 70 kg. It has beneficial actions in epilepsy, hypertension, congestive heart failure, liver, eyes and in some others. Its preventing role is increasing in various life threaten diseases. Bone loss in women is an old age problem where it has helping hand. It has been patented for several symptoms and diseases and found to have clinical utility. But being an amino acid, therapeutic use confronts limitations; restricted permeability, higher doses and many more; necessitate the relook for the development of pro-drugs (analogues) of taurine exploiting various structural alterations in carbon chain, amino and sulfonic ends. A large number of taurine derivatives have been reported with partial to marked activity. Taurine derivatives like taltarimide, acomprosate and tauromustine are already in use as anticonvulsant, anti-alcoholic and anti cancer agents. Taurine is now part of several energy drinks, functional food, nutriceuticals, and anti-ageing formulas. The in depth analysis of these analogues and their biological actions can provide certain clues for further consideration. In this presentation, attempts have been made to provide synopsis, synthesis and symbiosis of its chemical and biological actions, which may facilitate further research in this area. The successful journey of these heterocycles to clinical utility is a healthy and happy sign and an index of bright future in alleviating such suffering.

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TRANSITION METAL COMPLEXES/ORGANOMETALLIC COMPOUNDS AS ANTICANCER/ANTI HIV DRUGS IN PHARMACEUTICAL INDUSTRY

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Cancer is a dreadful disease and any practical solution in combating this disease is of paramount importance to public health. Cancer patients have burdened by drug induced toxic side effects, and no one turned to seek help from the complementary and alternative medicine hoping for a better cure. Research on platinum based drugs and non-platinum based drugs is a multi-million dollar industry in USA and there is every need to produce safe drugs for the cure of this monstrous disease. Flavonoids have a long history of use in traditional medicines in many cultures. The phytochemical, curcumin is one of the major dietary flavonoid, belonging to a group of flavonol. Curcumin is a natural polyphenol. It is highly potential molecule capable of preventing and treating various cancers. Various dietary chemo preventive agents, turmeric powder or its extract are broadly used as therapeutic preparations in Indian system of medicine. We provide a summarized synthesis and structural determination of curcumin oxime, curcumin thiosemicarbazone derivative of gold (III) complex. These analogs are used for prevention of cancer tumor progression and treatment of human malignancies. A pharmacologic agent is observed for treating and/or preventing cancer, among other diseases and conditions, and particularly breast, prostate, and pancreatic cancer, in humans and animals. The novel pharmacologic agent is an isoflavonoid or isoflavonoid mimetic covalently attached to a cytotoxic pharmacophore that, preferably has the ability to conjugate with a metal salt to form a more potent metal complex, particularly a Au (III) complex and other complexes of platinum, palladium, ruthenium, copper etc. My talk would mainly encompass different transition metal complexes/organometallic compounds that are presently used as drugs, especially anticancer and anti-HIV drugs, apart from anti-inflammatory, antimicrobial, antibacterial and diseases like arthritis and Parkinson's disease etc. The talk would mainly focus on the use of medicinal chemistry and its application to drug design and development in pharmaceutical industry, especially transition metal complexes and organometallic compounds viz. gold, platinum, palladium and ruthenium apart from copper, cobalt, iron, nickel, zinc, cadmium etc. The main emphasis of my talk would be on different class of ligands, their Schiff's bases and transition metal complexes especially Au, Pt, Pd and Ru, with the main aim of designing, developing very novel small molecules, as possible and extremely potential candidates as anti-cancer and anti-HIV drugs. The talk would provide an overview of current programs being undertaken in our laboratories, especially focused on the development of potent ligands capable of recognizing binding sites and diverse strategies employed by my group for elucidation of anti-cancer and anti-HIV drug leads to circumvent the problem caused by cis-platin. We have synthesized and characterized several phytochemicals from traditional medicinal plants and isolated some phytochemicals and made the corresponding oximes, thiosemicarbazones and substituted thiosemicarbazones as ligands and synthesized, characterized, structurally elucidated their transition metal complexes especially with gold, platinum, palladium, ruthenium, copper etc. and studied their anticancer activity, nuclease activity etc. and tested their potential as anticancer drugs. The main aim of our extensive/preclinical pharmaceutical development program is to investigate the use of these extremely novel small molecules-metal complexes/compounds of phytochemicals, flavanoids etc., which have very interesting structural features and properties and hence are excellent candidates as anti-cancer and anti-HIV drugs. The main aim of our research is design, development and synthesis of transition metal complexes/organometallic compounds that would certainly help to bring this force of nature from bench to bedside and enhance cancer killing with less toxic effects and would certainly lead to initiation of clinical trials.

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21ST CENTURY DRUG DELIVERY WILL TRANSFORM HEALTHCARE: OPPORTUNITIES FOR NANOSCIENCE AND CHEMISTRY

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The pre-human ancestors improved eating habit to develop brain by roasting food million years ago. Food consumed by this method remained contaminated with charred carbon. Such a practice is now translated in barbeque type delicacies. We have shown that these charred carbon associated with roasted food essentially comprised of non-toxic graphene and nano carbon materials to sustain human endeavor. It was discovered that metamorphism of plants leading to coalification naturally create graphene oxide(GO) sheets under 100x100 nm size and such GOs are isolated from low grade coal. Irrespective of the source of isolation, these GOs are shown to be non-toxic and fluorescing in the entire three red green and blue regions. Living images of laboratory animals in their entire life cycle have been demonstrated using *Drosophila melanaogaster* as the proof of concept to use these nanocarbons in bio-medical research. These water soluble corrugated type GO sheets can reversibly close like spheres and re-open up to sheet forms based on chemical and physical stimuli as code similar to, "close and open sesame diktat" used in folk tale, Alibaba and forty thieves' . Based on such property, these nano carbons are used as cargo (Trojan horse) to carry drug like Donepezil (for Alzheimer), Taxol (for cancer) and hydrophobic porphyrin (for PDT therapy). The solubility of the entrapped drug follows the property of the cargo as these become now soluble in aqueous PBS buffer differing insoluble behavior in their free state. Such solubility property of the entrapped drug thus bypasses the problem in administrating insoluble drug. We use this probe to show that these can cross blood brain barrier in mice model and reach in the neuronal site of the brain. Finally the empty cargo can safely be excreted from the body. We will briefly touch our ongoing research to entrap insulin using this cargo for room temperature storage stability and its oral administration in diabetes patient.

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SYNTHESIS OF A MOLECULAR IMPRINTED POLYMER AS AN ABSORBENT FOR SELECTIVE EXTRACTION OF A TRIAZINE HERBICIDE FROM BIOLOGICAL SAMPLES

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Background & Aim: Increasing production and the use of pesticides for agricultural purposes can lead to many environmental and human health risks. Therefore, trace residue analysis and the assessment of their concentration in occupational and environmental samples is highly necessary to estimate human exposure levels. This study was aimed to use a synthesized molecular imprinted polymer (MIP) as a novel and specific absorbent for residue analysis of metribuzin herbicide in biological sample.

Method: The MIP was synthesized by copolymerizing the named pesticide as the template molecule in presence of methacrylic acid and ethylene glycol dimethacrylate as functional and crosslinking monomers, respectively. Afterwards, important parameters affecting the adsorption and recycling process of metribuzin were optimized using synthesized absorbent through the solid phase extraction (SPE) method to demonstrate the ability of the synthesized MIP for selective recognition of analyte of interest from biological sample. All samples were then analysed by high performance liquid chromatography.

Results: According to the obtained results, trace amount of herbicide of interest was successfully determined using synthesized MIP. The optimum amounts of effective parameters on extraction yield were determined as follow: adsorbent amount-13.15 mg, sample pH-3, sample flow rate-1 mL /min, volume of extraction solvent-1.33 mL, flow rate of extraction solvent-3 ml/min, and the amount of acid in the solvent composition-10%. Detection and quantification limits of the method were 0.0119 and 0.0397 ppb, respectively.

Conclusion: The developed method can be used as an optimum sample preparation procedure for selective and sensitive extraction procedure and determination of desired herbicide from biological sample.

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NUCLEOPHILIC C-H FUNCTIONALIZATION OF ARENES: A NEW SYNTHETIC TOOL FOR GREEN CHEMISTRY

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Direct metal-free C-H functionalization of aromatic and heteroaromatic compounds is a new chapter in organic chemistry. The results of comprehensive studies on nucleophilic substitution of hydrogen in arenes and hetarenes (the SNH reactions), including their mechanisms, intermediates, mathematic and electrochemical modeling, kinetics, electron-transfer, etc. will be presented and discussed. The SNH methodology is of great practical value, since it involves nucleophilic alkylation, alkenylation, alkynylation, arylation, amination, hydroxylation, alkoxylation, cyanation, cyanomethylation, halogenation, as well as cymantrenylation, carboranylation, ferrocenylation and other reactions. The SNH reactions change the logic of organic synthesis, providing a powerful synthetic tool to functionalize C-H chemical bonds in a variety of nitro- and azaaromatic compounds, quinones, azinones, porphyrins, azulenes and arene-metal-complexes. Also they can be carried out in the electrochemical mode, which opens new opportunities to avoid preliminary incorporation of good leaving groups or other functionalities in an aromatic ring, thus being in a good agreement with principles of green chemistry.

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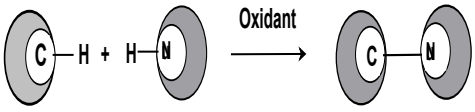

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INVOLVING UNDERGRADUATE STUDENTS IN THE RESEARCH OF ASSESSING AND IMPROVING THE SCIENTIFIC EXPLANATION ABILITY OF AMERICAN UNDERGRADUATE STUDENTS IN GENERAL CHEMISTRY CLASSES

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Despite the call by the US National Research Council for college students to construct and defend their explanations, many college students are unable to construct sufficient scientific explanations even for concepts they feel they understand. This SoTL research involves current undergraduate students and seeks to answer the following research questions in the setting of General Chemistry I lectures in a medium sized public university in US: 1) What are some good methods of instructing students to construct sufficient scientific explanations? 2) How does the practice of constructing scientific explanations affect the students understanding of the concepts involved? The pilot study conducted in Fall 2017 suggested that, teaching students a systematic way of constructing scientific explanations through short online video assignments based on Toulmin's Argumentation Pattern, together with the consistent practice of constructing scientific explanations in daily homework assignments, had a positive and statistically significant impact on students' overall understanding of course materials. It was measured by multiple assessment tools, including the ACS standardized exam where the treatment group scored an average of 71st percentile as opposed to the average of 32nd percentile scored by the control group. To continue this study at a larger scale, a series of short video assignments can be designed and administered to a larger size of treatment group. If these interventions continue to bring positive impacts, they can be administered to general chemistry classes in other universities. Similar videos can be designed to improve students' understandings in upper level chemistry classes as well.

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FABRICATION OF MAGNETIC IRON ENRICHED BIOCHAR NANO-COMPOSITE: EFFECTIVE PHOSPHATE RECOVERY FROM ANAEROBIC DIGESTED SWINE SLURRY AND INFLUENCING FACTORS

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The fabrication of magnetic iron enriched biochar nano-composite and its further use as an adsorbent to recover phosphate from liquid fractions of anaerobic digestate were comparatively evaluated in this study. The raw biochars (Coconut Shell and Wheat) were magnetically modified through their dissolution in $FeCl_3.nH_2OFeSO_4$ and $Fe_2(SO_4)_3.nH2O$ (n=6 to 9). The comparative performance evaluation between pristine (Coconut shell biochar, CCB; Wheat biochar, WHB) and magnetically modified biochars (Coconut shell magnetic biochar, CCMB; Wheat magnetic biochar, WHMB) was investigated through a series of batch experiment. Magnetic Fe biochar surface modification showed a decrease of negative charge as well as surface area properties of CCMB and WHMB. Obtained results indicate that, magnetically modified biochars showed remarkable adsorption performance CCMB and WHMB (33.27 and 29.71 $mg.g^{-1}$) due to positive charge built up onto the surface of modified chars rather than CCB and WHB (17.57 and 15.21 $mg.g^{-1}$). The nature of PO_4^{3-} sorption for modified and unmodified chars confirmed to the Pseudo 2nd order (R^2 = 0.999, 0.999, 0.999, 0.998–0.998, 0.999, 0.998, 0.999). The isotherm data was better fitted to the Langmuir and Freundlich model (R^2= 0.967, 0.960, 0.987, 0.946)-(0.983, 0.983, 0.997, 0.997). The characterization results (XRD, SEM, and FTIR) showed that multiple sorption mechanism was involved during adsorption process. The dominant PO_4^{3-} sorption pathway to CCMB and WHMB was electrostatic attraction, surface precipitation rather than unmodified chars where electrostatic attraction was dominant. Thermodynamically, spontaneous and endothermic PO_4^{3-} adsorption mechanism in solution and liquid digestate was mainly associated with dipole dipole and hydrogen bonding force. Furthermore, the regenerated MBCs retained the substantial PO_4^{3-} adsorption capacity upto several time of regeneration cycles. Thus, obtained results herein suggest that these materials could be employed as a potential filter to recover nutrients from contaminated matrix.

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