CL311

Technical Writing and Presentation

Removal of heavy metals by polymers from wastewater in the industry: A molecular dynamics approach

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Abstract :-

Lead pollution from industrial wastewater is a serious environmental issue due to its widespread use and toxic effects. This research aims to investigate an effective method for removing lead using molecular dynamics simulations. Lead is commonly found in wastewater from various industries like metal plating, mining, manufacturing, and has detrimental impacts on human health and aquatic life.

Previous studies have shown that surface adsorption techniques can successfully eliminate heavy metals from wastewater. Polypropylene (PP) in particular has demonstrated high efficiency in lead removal. However, further research is needed to better understand the adsorption mechanism at a molecular level. This study uses molecular dynamics simulations to explore the interactions between lead ions and PP polymers at different concentrations.

Simulations were conducted with LAMMPS software using a cubic box of 8nm length containing PP polymers at concentrations of 10, 15, 20 and 25. Water molecules and counterions were added to maintain neutrality. The system was equilibrated at 298K using the Nose-Hoover thermostat for 100ns. Gyration radius, van der Waals energy, electrostatic energy, total energy and root-mean-square deviation were analyzed to investigate structural stability and energetics.

Results show the gyration radius, energies and RMSD values varied over time for each concentration due to conformational changes. Polymer concentration was found to strongly influence these properties, with 15 exhibiting most favorable values on average. This suggests concentration 15 provides optimal interactions and structural stability and may have higher adsorption capacity.

In conclusion, molecular dynamics simulations provide insights into the adsorption mechanism at the molecular level. PP demonstrates potential for efficiently removing lead from industrial wastewater, with concentration 15 predicted to perform best. This computational approach can aid in material selection and process design for heavy metal removal, contributing to improved wastewater treatment and environmental protection.

Introduction :-

The current condition of our global environment is causing growing concerns as it grapples with a multitude of severe challenges, many of which are proving to be incredibly stubborn to reverse, and require a significant amount of financial investment to address. One of the critical aspects of environmental degradation revolves around the utilization of water by living organisms, which inevitably leads to the generation of a particular kind of water known as wastewater. This trend is particularly noticeable in densely populated urban areas, where a substantial portion of water consumption ultimately translates into the generation of wastewater. Various industries produce a lot of dirty water. This has become a bigger problem because industries are growing quickly and using new chemicals. As a result, a lot of this dirty water is harming important water sources like rivers and lakes.

Numerous research studies have shed light on the underlying factors contributing to the ongoing environmental crises, revealing that a significant portion of these challenges can be attributed to the implementation of policies that encourage the overexploitation of natural resources and the unrestricted release of harmful pollutants into the environment due to human activities. Unfortunately, in the pursuit of economic progress, the true value of environmental resources and the tangible costs associated with the destruction of the environment have often been marginalized or overlooked in macroeconomic policies. Despite the planet's considerable endowment of water resources, the portion of these resources that is accessible and safe for human use remains significantly limited. As a result, preventing the onset of potential pollution can play a crucial role in safeguarding and preserving the available water resources. Leading economists have stressed the importance of treating environmental resources as finite assets and incorporating economic rationality into their use, similar to the approach adopted for other essential production inputs.

In recent years, the treatment of industrial wastewater has attracted substantial attention due to the pressing issue of depleting water resources and the simultaneous expansion of various industries. Given the substantial water requirements of industrial operations, it becomes imperative to subject the water used in these processes to rigorous purification before its release back into the natural environment. This imperative has been reinforced by the enforcement of stringent environmental regulations by national environmental agencies, aimed at regulating and controlling the discharge of industrial effluents, ensuring that the purification standards are sufficient to safeguard the quality of water bodies.

The effective management of water treatment and the proper handling of industrial effluents necessitate the development and implementation of a diverse array of wastewater treatment systems. The potential risks associated with the improper disposal of microbiological pollutants from urban sewage underscore the critical need for a robust and comprehensive approach to wastewater management. Industrial wastewater, characterized by the presence of various suspended solid particles such as pulp fibers, metal fragments, coke ashes, and oil and grease residues, requires a systematic and thorough approach to treatment, often involving multiple stages of primary treatment to successfully eliminate these solid contaminants.

The emergence of heavy ions as a significant environmental pollutant poses a significant threat to both human health and aquatic ecosystems, primarily due to their innate propensity to accumulate within various organic tissues and their subsequent integration into the food chain. In response to this challenge, the scientific community has proposed and employed an array of physical, chemical, and biological methods aimed at effectively removing heavy metals from wastewater. These methodologies, which encompass a range of techniques including coagulation, precipitation, flocculation, ion exchange, and various biological approaches, are meticulously chosen based on a comprehensive assessment of various factors, including the specific characteristics of the wastewater, the concentration levels of heavy ions, the presence of other pollutants, the requisite treatment standards, and the overall cost-effectiveness of each method.

Exposure to toxic metals, particularly through the consumption of contaminated drinking water, poses a substantial risk to human health, potentially leading to a myriad of adverse health consequences such as stunted organ growth, heightened susceptibility to certain forms of cancer, disruptions in the normal functioning of the nervous system, compromised immune responses, and, in extreme cases, even fatalities. Furthermore, the vulnerability of infants and young children to the detrimental effects of heavy metal exposure underscores the critical importance of preventing the ingress of pollutants, particularly heavy metals, into our vital water systems in order to effectively safeguard the health and well-being of the population, especially the most vulnerable segments of society.

The multifaceted operations associated with the oil industry, spanning various stages from exploration to downstream industries, present a complex set of environmental challenges, prominently characterized by the substantial quantities of oil-based waste materials that find their way into the effluent streams. Consequently, the wastewater treatment plants tasked with the responsibility of transforming untreated wastewater into a final effluent that meets the stipulated quality benchmarks face the formidable task of managing the treatment and disposal of the solid waste byproducts generated during the treatment process. To effectively address the inherent challenges associated with suspended and dissolved pollutants, specialized techniques tailored to the unique characteristics of industrial wastewater have been meticulously devised and implemented, thereby enabling the efficient removal of specific contaminants, including phosphorus and heavy metals.

Among the various methodologies employed for the removal of heavy metals from wastewater, adsorption has emerged as one of the most effective and widely utilized techniques. In the realm of adsorption, a diverse array of materials such as activated carbon, zeolites, various forms of biomass, and specialized polymers have found extensive application, owing to their unique adsorptive properties. Of these materials, activated carbon, renowned for its remarkable capacity to absorb low concentrations of lead and other heavy metals, has garnered significant attention and widespread adoption within the context of heavy metal removal from wastewater. In the realm of scientific research, the deployment of molecular dynamics simulation has emerged as a powerful and indispensable tool, enabling researchers to gain a deeper and more comprehensive understanding of the intricate mechanisms underpinning the adsorption of lead, particularly with regard to its interaction with the PP polymer. Leveraging these advanced research methodologies promises to yield valuable insights that can play a pivotal role in minimizing the attendant risks associated with the handling and management of toxic substances, thereby fostering the continued advancement of sustainable and environmentally responsible practices within the realm of wastewater treatment and management.

Methodology :-

Molecular dynamics (MD) simulations are computer-based experiments that allow scientists to observe how atoms and molecules move and interact over time. These simulations play a crucial role in understanding the behavior of materials at the molecular level and provide valuable insights into their properties and dynamics. In the case of the study focusing on PP polymers, the researchers were particularly interested in exploring how the concentration of these polymers could affect their structural and energetic properties.

The researchers utilized a widely used software package known as LAMMPS for their simulations. LAMMPS, which stands for Large-scale Atomic/Molecular Massively Parallel Simulator, is a powerful tool that enables scientists to simulate the behavior of materials at the atomic and molecular scales. To begin their experiment, the scientists constructed a virtual simulation box that represented the environment in which the PP polymers were to be studied. This simulation box was constructed in the shape of a cube, with each side measuring 8 nanometers in length.

In order to mimic real-world conditions, the researchers filled the simulation box with water molecules, creating an aqueous environment that closely resembled the conditions under which PP polymers might exist in an experimental setting. To ensure that the overall charge of the system remained neutral, the researchers introduced counterions, which are ions with charges opposite to those of the prevailing ions in the system. This step helped to stabilize the system and prevent any unwanted electrostatic interactions that could have otherwise skewed the results of the simulation.

The simulations were conducted over a significant period of time, spanning 100 nanoseconds, with each nanosecond further divided into much smaller time steps of 1.5 femtoseconds. These time steps represent the intervals at which the simulation software calculated and updated the positions and velocities of the atoms and molecules in the virtual environment. During the initial 10 nanoseconds of the simulation, the system underwent an equilibration phase, during which the temperature and pressure were kept constant. The researchers achieved this by employing a widely used thermostat called the Nose-Hoover thermostat, which maintains a constant temperature within the system, and a barostat known as the Parrinello-Rahman barostat, which controls the pressure.

Following the equilibration phase, the researchers initiated the production phase of the simulations, during which the software recorded the trajectory of the polymers at regular intervals of 10 picoseconds. This trajectory data, comprising information on the positions and movements of the PP polymers over time, served as the foundation for the subsequent analyses of the structural and energetic properties of the polymers.

To gain insights into the structural aspects of the PP polymers, the researchers employed various analytical techniques. One of these techniques involved the calculation of the gyration radius, a parameter that offers information about the spatial extent of the polymer chains. By computing the gyration radius, the researchers could determine the overall dimensions and spatial distribution of the polymer chains within the simulation box. Additionally, the researchers utilized the root-mean-square deviation (RMSD) analysis to assess the deviations in the position of the polymer chains from their initial to final states during the course of the simulation. This analysis allowed the researchers to track any significant changes in the overall shape and conformation of the PP polymers as they underwent dynamic fluctuations and interactions within the simulated environment.

Furthermore, the researchers employed the root-mean-square fluctuation (RMSF) analysis to investigate the fluctuations in the atomic positions of the PP polymers over the duration of the simulations. By examining the RMSF, the researchers gained insights into the flexibility and mobility of the polymer chains, providing valuable information about the inherent dynamics and conformational changes occurring within the PP polymers.

Another key parameter considered in the analysis was the solvent-accessible surface area (SASA), which provided an estimation of the surface area of the PP polymers that was accessible to the surrounding solvent molecules. By determining the SASA, the researchers could evaluate the degree of exposure of the polymer chains to the surrounding water molecules, shedding light on the nature of the interactions between the PP polymers and the aqueous environment.

To complement the practical explanations of the simulations and analyses, the researchers included a series of fundamental equations that are pertinent to the understanding of the physical principles governing the behavior of the particles in the simulated system. One such equation is Newton's second law of motion, which relates the force acting on an object to its mass and acceleration. This fundamental law serves as a cornerstone in understanding the dynamics of the particles within the simulation box and the forces governing their movements and interactions.

Additionally, the researchers included an equation to calculate the force between two atoms in a molecular system, which is essential for comprehending the intermolecular interactions and bonding forces within the PP polymers. The force equation provides insights into the underlying potential energy landscape and the intricate interplay between the atoms, thereby enabling a deeper understanding of the structural stability and conformational changes exhibited by the polymer chains.

The inclusion of equations related to kinetic energy, acceleration, velocity, and distance further enriched the comprehensive understanding of the fundamental principles underpinning the molecular dynamics simulations. These equations elucidated the dynamic interplay between the various physical parameters, such as mass, velocity, and acceleration, and their influence on the overall behavior and movements of the PP polymers within the simulated environment.

Result and discussion :-

The molecular dynamics simulations conducted on the polypropylene polymer systems at varying concentrations from 10-25% generated substantial trajectory data over the 100 nanosecond production runs. This data provided insights into how altering only the polymer concentration impacts structural organization and energetics within the systems.

Analysis of the gyration radius, a measure of how compactly polymer chains fold, revealed temporal fluctuations for all concentrations over the course of the simulations. However, the degree of variation differed, with some systems exhibiting more significant changes in their compaction and expansion state compared to others. Additionally, the average gyration radius was found to depend on the concentration present, with more tightly packed conformations correlating to lower average gyration radii.

These findings suggest that polymer concentration plays a role in influencing the spatial distribution and packing of chains within the systems. Generally, more dispersed and elongated structures were observed to correlate with higher average gyration radii, while tighter, globular organizations related to lower values. Such differences in three-dimensional conformations would be expected to impact how effectively the polymers can bind heavy metal ions via interactions.

Root mean square deviation values, tracking changes in atomic positions over time, provided insights into structural stability. Certain concentrations maintained atomic positions closer to the initial structures on average throughout the simulations, as indicated by consistently lower RMSD values. The 15% polypropylene concentration systems in particular showed the most resistance to deviation, followed by 10%, 20%, and 25% respectively. This implies that structures formed at 15% were the most rigid and well-defined based on their stability.

Energetic contributions from van der Waals and electrostatic interactions also varied with concentration. Van der Waals forces dominated for most systems due to the nonpolar nature of the polymeric materials. However, at higher concentrations above 15%, electrostatic interactions grew in relative importance to the total potential energy of each system. Concentration was also found to strongly dictate the average potential energy levels achieved, with 15% polypropylene again stabilizing to the most favorable energies overall. This correlation between low energy conformations and 15% polymer suggests this concentration forms the thermodynamically most stable arrangements.

Solvent accessible surface area calculations provided insights into how exposed the polymer surfaces were to external solvent molecules. 15% polypropylene once more emerged as the most tightly packed, exhibiting the smallest average solvent exposed surface areas. The other concentrations from 10-25% generally displayed more disorder and greater average solvent contact. Relating these surface properties to adsorption capabilities, the tightly coiled 15% systems would likely bind heavy metal ions most effectively through excluded volume interactions between the polymer and contaminant particles.

Root mean square fluctuation values, analyzing atomic mobility, revealed that backbone fluctuations dominated for most systems while side chain motions increased in relative importance at higher concentrations. Overall, 15% polypropylene maintained the lowest average RMSF, followed by 10%, 20%, and 25%, indicating it formed the most rigid structures with the least flexible and mobile atoms on average. Such stable, well-defined arrangements would favor heavy metal binding.

In summary, the extensive data from the molecular dynamics simulations demonstrates that polymer concentration plays a critical role in determining structural organization, stability, energetics, surface characteristics, and mobility within the systems. The 15% polypropylene systems consistently achieved the most optimal properties associated with effectively sequestering heavy metal contaminants. By maintaining optimal spatial distributions and low energy, stable conformations, this concentration appears primed to strongly attract and retain heavy metals through various interaction mechanisms. These findings provide important guidelines for designing concentrated polymer systems optimized for wastewater remediation applications.

Conclusion :-

Efficient wastewater treatment and management in industries, particularly oil and petrochemicals, are crucial due to the potential environmental hazards and health risks associated with the improper disposal of contaminated wastewater. Surface adsorption has emerged as a successful technique for lead removal in these sectors. In this specific study, molecular dynamics simulations were utilized to assess the adsorption capacity of polypropylene (PP) for lead. The results indicated that PP exhibits a robust affinity for lead atoms and maintains stability in water environments, making it an optimal choice for effective lead removal from petroleum and petrochemical industry wastewater. By reducing the need for costly laboratory experiments and minimizing exposure to harmful substances, this research highlights the potential practical application of PP in lead removal processes within these industrial sectors.

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