2025. Volume 9, Number 1 Pages 10-15

UDC: 678.56+620.3
DOI: https://doi.org/10.30546/2521-6317.2025.01.463

INTEGRATION OF ASPEN PLUS AND NAMD FOR THE DESIGN AND OPTIMIZATION OF CHITOSAN-GRAPHENE OXIDE COMPOSITE HYDROGELS

Nizami AKBAROV[1], Narmina GULIYEVA[2*], Elsun AZIZOV[3], Rasul RAHIMOV[2], Zulfiya JAVADOVA[2], Narmin ISMAYILOVA[2]

Department of Analytical and Organic Chemistry, Azerbaijan State Pedagogical University, Baku, Azerbaijan

[2]Department of Chemical Engineering, Baku Engineering University, Baku, Azerbaijan
[3]Institute for Chemistry and Processes for Energy, the Environment and Health (ICPEES), University of Strasbourg, Strasbourg, France

ARTICLE INFO

Article history:
Received:2025-10-27
Received in revised form:2025-10-27
Accepted:2025-12-16
Available online

Keywords:
chitosan, Aspen Plus, NAMD, graphene oxide, nanomaterials, water purification, membranes, chemical engineering, environmental applications.

ABSTRACT

This study explores the use of Aspen Plus and NAMD as powerful tools for the simulation and design of processes using chitosan as a component and its functionalized derivatives. By employing these digital platforms, researchers can effectively analyze and predict the performance potential of chitosan-derived systems, especially in applications related to bioengineering and environmental science. Their implementation significantly reduces the risk of errors during synthesis and structuring, improves product yield, and facilitates further functionalization of materials. Particular attention is given to the utilization of (GO) graphene oxide in water treatment technologies. The paper outlines a method for synthesizing GO and investigates the structural and functional characteristics of its surface layers. It also discusses the integration of GO into chitosan-based matrices for the development of advanced membrane systems showing enhanced ability to filter impurities. Empirical evidence proves that the application of digital modeling tools contributes to the optimization of research and development processes involving chitosan and (GO) graphene oxide, supporting the creation of innovative materials for environmental engineering purposes.

**Corresponding author:*
Narmina A. Guliyeva, e-mail: nquliyeva@beu.edu.az

INTRODUCTION

Aspen Plus is widely used in engineering and industry for optimization and design of chemical processes. Its capabilities include: process design, equipment modeling and simulation, environmental analysis, big data integration [1]. Aspen Plus is ideal for solving large-scale problems that require the consideration of aggregated properties of materials and systems [2]. NAMD (“Nanoscale Molecular Dynamics”) is used in molecular dynamics to simulate the behavior of atoms and molecules. Key capabilities of NAMD include: biomolecular research, materials science, high performance computing, integration with visualizers [3]. NAMD is in demand in academic research, pharmaceuticals and materials science, where atomic level detail is important [4]. Despite the differences in modeling scale, Aspen Plus and NAMD can complement each other. The use of Aspen Plus and NAMD continues to expand due to the following trends in biotechnology and organic synthesis to produce composite materials for medical and food engineering applications. Both approaches are crucial in fostering innovation within the field of sustainable materials and environmentally sound technologies. Chitosan, obtained by deacetylation of chitin, is a an altered form of a natural polysaccharide possessing remarkable physical, chemical, and biological characteristics, notably biocompatibility, biodegradability, and fat-binding ability, heavy metals, and other substances [5]. Structurally, chitosan consists of repeating units of 2-amino-2-deoxy-D-glucose linked by β-(1→4)-glycosidic bonds, which forms its polymer framework [6]. The polymer structure of chitosan is due to the presence of amino groups in the C2 position, which, depending on the degree of deacetylation and pH of the medium, can be in a protonated or neutral form. This feature determines such key properties of chitosan as the ability to ion exchange and interact with charged molecules, including proteins, lipids, and organic acids. Additionally, the existence of both amino and hydroxyl groups in the chitosan backbone contributes to its elevated reactivity, positioning it as a versatile platform for functionalization and composite formation. For example, modification of the polymer chain allows obtaining derivatives with specified properties, such as improved solubility, sorption capacity or specific bioactivity.

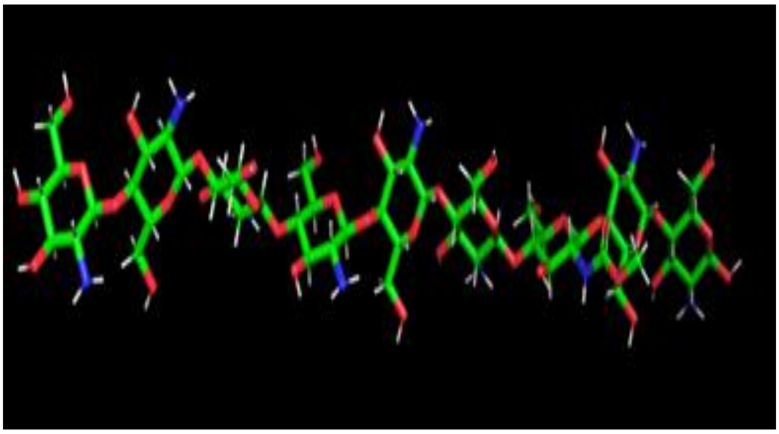

Fig.1. Molecular structure of chitosan visualized using the NAMD program.

The conformational features of chitosan, including the spatial arrangement of acetyl groups in N-acetylglucosamine units, plays an important role in predicting its behavior in various chemical and biological systems [7]. Chitosan possesses distinctive properties that make it increasingly sought after across various industries. Its market potential is expected to expand, driven by global trends such as environmental awareness, the pursuit of healthier lifestyles, and advancements in innovative technologies. In healthcare and medicine, chitosan is gaining traction due to its natural origins and beneficial characteristics.These aspects are the subject of active research in the field of synthesis of new materials, biomedicine and environmental cleaning technologies [8]. As an ingredient in dietary supplements, chitosan is valued for its ability to lower cholesterol, enhance metabolism, and support gut health. Marketing efforts will focus on highlighting its natural composition, safety, and positive effects on overall well-being. Thanks to its antimicrobial, anti-inflammatory, and wound-healing properties, chitosan is also widely applied in medical products, such as dressings, surgical sutures, and antibacterial coatings. The promotion of these materials will underscore their eco-friendly nature, efficiency, and compatibility with biological systems, supported by technologies like ASPEN PLUS and

NAMD. In agriculture, chitosan is utilized as a biopesticide and plant growth enhancer. Its capacity to strengthen plant immunity and increase resilience to stress positions it as a promising tool in promoting organic and sustainable farming practices [9]. Chitosan is very popular in the food industry because it is practically not absorbed in the gastrointestinal tract [10], which makes it a valuable component for the production of low-calorie products, serves as a source of essential substances and improves the technological properties of food products. Its ability to bind and remove fats and toxins from the body, as well as its minimal caloric content, make chitosan indispensable for the creation of healthy food products and health maintenance products [11,12]. The versatility of GO also extends beyond environmental applications. Its layered structure and the potential for functional group modification make it an invaluable material in biomedicine, engineering, and technology. These applications leverage the ability of GO to form a range of covalent and non-covalent bonds through its functional groups, further broadening its utility [13,14]. The oxygen content in graphene oxide, which typically ranges from 3% to 40% by weight, significantly influences its properties. A precise understanding of the oxygen-functional group content is essential for optimizing GO's performance in various applications [15,16]. Furthermore, the composition of GO can vary with changes in its surface area, which directly impacts its adsorption efficiency and reactivity. Research has demonstrated that GO membranes exhibit exceptional water permeability combined with selective ion and molecule transport, making them highly effective in water filtration systems.

In the field of nanotechnology, GO is increasingly recognized as a cost-effective and environmentally friendly material for purifying water from toxic pollutants [17,18]. Its applications range from sewage treatment and CO2 capture to the removal of residual pesticides and pharmaceuticals from water, showcasing its adaptability and effectiveness [19,20]. The continuous exploration of GO's properties and its integration into innovative technologies highlight its potential to transform environmental protection strategies while contributing to sustainable development goals [16,18,20].

EXPERIMENTAL PART

- Preparation of Chitosan-Based Hydrogels Using Different Concentrated Solutions

Chitosan was dissolved in acetic acid solution (0.1%) and stirred for several hours to ensure complete dissolution of chitosan. The prepared gel was then placed in Petri dishes with a thickness of approximately 3-6 mm. NaOH solution (1-5 M) was slowly added to the chitosan solution, forming gels with different textures according to the different concentrations of the solutions.

- Method for Synthesis of Graphene Oxide

For the synthesis of graphene oxide, three plastic containers were prepared, each containing 3 g of graphite and 1 g of sodium nitrate ($NaNO_3$) and 6 g of potassium permanganate ($KMnO_4$), respectively. Separately, 46 ml of concentrated sulfuric acid (95–98% H_2SO_4) was measured out using a graduated cylinder. To monitor the exothermic reaction, the process was carried out in an ice bath using multi-necked flasks equipped with thermometers to maintain precise temperature control. $KMnO_4$ was added slowly over two hours, ensuring that the reaction temperature remained within 20–25 °C. After continuous stirring for four hours, the resulting mixture was filtered, and the resulting solid product was thoroughly washed with distilled water to remove residual sulfuric acid and normalize the medium.

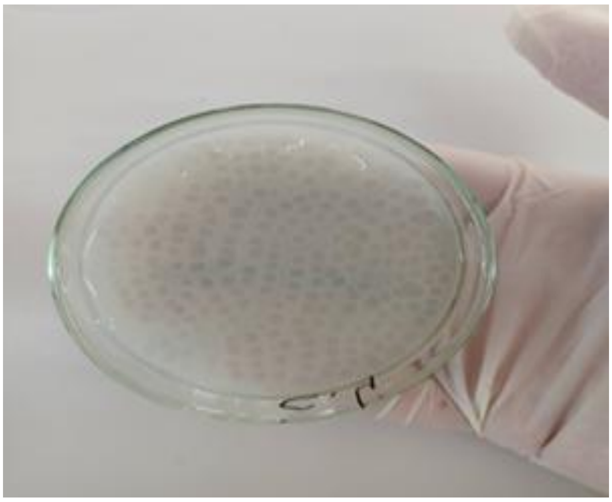

Fig. 2. Obtaining a hydrogel structure of chitosan

Fig. 3. Chitosan-based hydrogel for use in water purification

RESULTS AND DISCUSSION

This study uses an integrated approach combining numerical modeling and laboratory experiment to obtain and analyze a composite hydrogel based on functionalized chitosan and graphene oxide (Ch@GO). Modeling was performed using the Aspen Plus V12 and NAMD 2.14 software packages, which allowed us to cover both the macroscopic and molecular levels of interaction between the components.

- **Modeling in Aspen Plus**

The following parameters were varied during the modeling process: temperature (20–80 °C), pressure (atmospheric and elevated), mass ratio of components (chitosan, graphene oxide, acid solution), and the duration of ultrasonic treatment.

- **Molecular modeling in NAMD**

At the molecular level, the interaction between chitosan and graphene oxide was modeled using the NAMD package to describe the polysaccharide chains of chitosan and the functional groups of graphene oxide. The structures were considered at different pH values. The analysis showed stable formation of hydrogen bonds between the amino groups of chitosan and oxygen-containing groups of graphene oxide, with an average length of ~2.1 Å. With increasing pH, an increase in the distance between the chitosan chains was observed due to deionization, which potentially affects the degree of swelling and permeability of the hydrogel.

Experimental confirmation

To confirm the model data, laboratory experiments were carried out to synthesize a composite hydrogel. Mixtures of functionalized chitosan and graphene oxide (Ch@GO) were prepared in weight ratios of 1:1, 2:1 and 3:1. Chitosan was dissolved in 0.1% acetic acid solution with stirring, after which graphene oxide was added. The resulting solutions were treated with an ultrasonic device until a homogeneous mass was obtained. The mixtures were poured into Petri dishes and kept at 50 ° C for 3 hours. The obtained samples demonstrated good form-forming properties, a homogeneous structure and high stability. The morphology and distribution of components in the composite corresponded to the structures predicted based on molecular modeling. Thus, the correspondence between the calculations and the actual properties of the synthesized material was experimentally confirmed. The use of numerical modeling made it possible to significantly narrow the range of experimental search and ensure the production of a hydrogel with predicted characteristics, underscoring the role of simulation-based approaches in optimizing all steps of composite biomaterial creation.

Fig.4. Chitosan-based graphene oxide (Ch@GO) hydrogel.

CONCLUSION

Aspen Plus and NAMD are powerful tools for exploring chitosan and its practical applications. The composite material and chitosan-based hydrogels can be used to effectively remove pollutants, which is important for environmental and industrial applications. The successful integration of molecular modeling and experimental methods confirms the promise of the approach for the development of new materials. The results can be scaled up for industrial production of filter systems and purification plants. In this study, we successfully synthesized a composite hydrogel comprising graphene oxide (GO) and chitosan, demonstrating its high potential for addressing water pollution issues. Structural refinement and performance enhancement of the chitosan-GO system were achieved through a combined computational approach using NAMD for molecular-level understanding and Aspen Plus for process-level modeling. This integrative methodology not only provided an optimized material design but also facilitated the evaluation of its scalability for environmental remediation applications. The comparison between these two modeling platforms highlights a promising path for the development and industrialization of advanced filtration materials based on biopolymer composites.

REFERENCES

1. Volin YM, Ostrovskii GM. Three phases in the development of computer simulation of chemical engineering systems. *Theoretical Foundations of Chemical Engineering*. 2006;40:281–290.
2. Shevyrev SA. Application of the Aspen Plus software package for simulation of the synthesis-gas composition in oxygen-free steam gasification of biomass. *Thermal Engineering*. 2021;68(9):698–704.
3. Kale LV, Skeel RD, Bhandarkar M, et al. NAMD: A parallel object-oriented molecular dynamics program. *International Journal of High Performance Computing Applications*. 1999;13(1):61–69.
4. Phillips JC, Braun R, Wang W, et al. Scalable molecular dynamics with NAMD. *Journal of Computational Chemistry*. 2005;26(16):1781–1802.
5. Guliyeva NA. Stability of water HKUST-1 upon mixing with chitosan and graphene oxide. *GFZ Conference Proceedings*. 2022/2025. Available from: https://gfz2025.sciencesconf.org/data/pages/03_Programme_de_taille_2026.pdf
6. Azad AK, Sermsintham N, Chandrkrachang S, Stevens WF. Chitosan membrane as a wound healing dressing: characterization and clinical application. *Journal of Biomedical Materials Research Part B: Applied Biomaterials*. 2004;69B:216–222.
7. Aziz MA, Cabral JD, Brooks HJL, et al. Antimicrobial properties of a chitosan dextran based hydrogel for surgical use. *Antimicrobial Agents and Chemotherapy*. 2012;56:280–287.
8. Arteche Pujana M, Pérez Álvarez L, Cesteros Iturbe LC, Katime I. Biodegradable chitosan nanogels crosslinked with genipin. *Carbohydrate Polymers*. 2013;94:836–842.
9. Kean T, Thanou M. Biodegradation, biodistribution and toxicity of chitosan. *Advanced Drug Delivery Reviews*. 2010;62:3–11.
10. Raafat D, Von Bargen K, Haas A, Sahl HG. Insights into the mode of action of chitosan as an antibacterial compound. *Applied and Environmental Microbiology*. 2008;74:3764–3773.
11. Miguel SP, Ribeiro MP, Brancal H, et al. Thermoresponsive chitosan–agarose hydrogel for skin regeneration. *Carbohydrate Polymers*. 2014;111:366–373.
12. Vissarionov SV, Asadulaev MS, Shabunin AS. Experimental evaluation of the efficiency of chitosan matrixes under conditions of modeling of bone defect in vivo. *Pediatric Traumatology, Orthopaedics and Reconstructive Surgery*. 2020;8(1):53–62. DOI: 10.17816/PTORS16480
13. Devi SC, Khan RA. Effect of graphene oxide on mechanical and durability performance of concrete. *Journal of Building Engineering*. 2020;27:100948.
14. Liu Z. Nonlinear optical properties of graphene oxide in nanosecond and picosecond regimes. *Applied Physics Letters*. 2009;94:021902.
15. Zheng X, Jia B, Chen X, Gu M. In situ third-order non-linear responses during laser reduction of graphene oxide thin films towards on-chip non-linear photonic devices. *Advanced Materials*. 2014;26(17):2699–2703.
16. Guliyeva NA, Abaszadea RG, Khanmammadova EA, Azizov EM. Synthesis and analysis of nanostructured graphene oxide. *Journal of Optoelectronic and Biomedical Materials*. 2023;15(1):23–30.
17. Akbarov NA, Guliyeva NA. Fertilizer based on graphene oxide nanolayers and nutrients from organic waste. *International Scientific Journal "Endless Light in Science"*. 2024:242–245.
18. Guliyeva NA, Azizov EM. Composite based on chitosan and graphene oxide. *International Journal of Sciences: Basic and Applied Research (IJSBAR)*. 2022;65(1):141–147.
19. Murshudov T, Elshan A, Asadov M, Guliyeva N, Rahimov M, Elsun A. Iron nanoparticle-containing graphene oxide: Synthesis and membrane properties. *Journal of Optoelectronic and Biomedical Materials*. 2025;17(2):119–127.
20. Massart R. Preparation of aqueous magnetic liquids in alkaline and acidic media. *IEEE Transactions on Magnetics*. 1981;17(2):1247–1248. DOI: 10.1109/TMAG.1981.1061188