Research on the Application System of Graphene Oil-Water Separation Process Simulation and Computer Simulation Technology

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Abstract. This paper proposes a graphene oil-water separation process simulation and computer simulation technology application system based on deep learning. First, a physical model describing the graphene oil-water separation process is established, taking into account factors such as fluid flow, interfacial tension, and capillary action. Corresponding mathematical equations, such as the Navier-Stokes equation and the Young-Laplace equation, are derived to describe the various physical quantities in the oil-water separation process. Through reasonable assumption and simplification, the paper can reduce the computational complexity of model and guarantee its solvability. In terms of simulation system design, a simulation platform based on FEA and CFD is constructed, including pre-processing, solving, and post-processing modules. The mathematical model is discretized using the finite element method, and numerical simulation is realized using simulation software such as ANSYS and COMSOL. A user-friendly interface is developed to facilitate users to input parameters, set simulation conditions, and visualize simulation results. In this paper, an experimental platform for the graphene oil-water separation process is built in a laboratory environment, and necessary instruments and equipment are configured. The oil-water separation experiment under different conditions was designed, and the performance indicators of graphene materials such as separation efficiency and stability were tested. These data are obtained by experiments, which are input to simulation system. A comparison was made between experimental results and simulation results, which proved that the model was correct. Experimental results show that this simulation system is effective in predicting the performance of graphene oil-water separation process and provides strong support for practical applications.

Keywords: Graphene, oil-water separation, process simulation, computer simulation, deep learning.

1. Introduction

With the acceleration of industrialization, oil-water separation technology plays a vital role in environmental protection, energy development and industrial production. In recent years, as a new type of two-dimensional material, graphene has shown great application potential in the field of oil-water separation due to its excellent physical and chemical properties such as ultra-high specific surface area, excellent conductivity, chemical stability and mechanical strength. Graphene-based composite materials can effectively utilize their hydrophilic/hydrophobic properties for oil-water separation, thereby achieving efficient water pollution control and resource recovery. However, most of the existing research focuses on the preparation of graphene materials and their basic performance analysis, and the dynamic simulation and computer simulation technology of graphene oil-water separation process have not been deeply studied. The research on graphene oil-water separation technology aims to quantitatively analyze and predict its separation mechanism by constructing a mathematical model of the graphene oil-water separation process [1]. By means of computer simulation technology, it is possible to analyze and optimize the key factors such as separation efficiency, reaction time and operation conditions. It is helpful to improve the efficiency and stability of separation technology, provide theoretical support for practical application in fields such as environment protection, petrochemicals and so on [2]. By establishing simulation and simulation models, researchers can have a clearer understanding of the physical and chemical processes in the graphene oil-water separation process, providing a strong reference for future experimental research and industrial applications.

The main goal of this study is to establish a mathematical model that can accurately describe the graphene oil-water separation process, and based on this model, design and implement a computer simulation system to predict and optimize the performance of oil-water separation [3]. Through this system, researchers can deeply analyze the factors that affect the separation efficiency and provide optimization strategies [4]. The implementation of this simulation system not only provides a theoretical basis for the further development of graphene oil-water separation technology, but also provides an operational technical solution for practical problems in industrial applications.

2. Construction of mathematical model of graphene oil-water separation process

This paper will discuss the physical model of graphene oil-water separation process and construct the corresponding mathematical equation based on the physical model [5]. The unique surface properties of graphene materials give it excellent performance in oil-water separation, but to achieve a comprehensive understanding of its separation process, multiple factors such as fluid flow, interfacial tension, and capillary action must be considered comprehensively. The following content will introduce the mathematical modeling of these factors and the derivation of corresponding formulas in detail.

2.1. Physical model

The physical phenomena in the graphene oil-water separation process mainly include oil-water interface interaction, capillary action, fluid flow, etc. The core mechanism of oil-water separation is the interaction between liquid molecules and graphene surface [6]. By regulating the hydrophilic/hydrophobic properties of graphene surface, the oil and water phases can be effectively separated. The fluid flow in the oil-water separation process can be described by the Navier-Stokes equation. Fluid flow is not only affected by external forces, but also driven by interfacial tension and capillary forces. Under the effect of capillary action, liquid flow rate changes on graphene surface, which influences separation efficiency. The interface tension is an important factor that influences oil-water separation efficiency [7]. During the process of oil-water separation, the morphological changes of oil-water interface affect the process of separation. The Young-Laplace equation is able to describe the pressure distribution at the interface of oil and water, so it can be used to analyze mechanical behavior during separation. Capillary action refers to the flow of liquid through pores. The pore structure of graphene has a close relationship with capillary force in graphene separation process, which influences the rate and effect of separation [8]. Capillary force is not only affected by the surface tension of the liquid, but also closely related to factors such as pore size and wettability of the liquid.

2.2. Mathematical model construction

According to the above physical phenomena, mathematical models are constructed in this paper based on relevant theory. In this model, the relation between fluid flow, interface tension and capillary action is described.

(1) Fluid flow equation

The fluid flow process follows the Navier-Stokes equation, which is expressed as:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=-\nabla p+\mu\nabla^2\mathbf{u}+\mathbf{F} \tag{1}$$

ρ is the fluid density, $\mathbf{u}$ is the fluid velocity, μ is the fluid viscosity, p is the fluid pressure, and $\mathbf{F}$ is the external force. In the course of oil and water separation, not only depends on the physical parameters, but also on the interface tension and capillary action [9]. Therefore, it is necessary to introduce the interfacial tension and capillary force terms into the Navier-Stokes equation.

(2) Oil-water interface pressure equation (Young-Laplace equation)

The pressure difference at the oil-water interface is a key factor affecting the separation efficiency. The Young-Laplace equation describes the pressure distribution of the liquid on the surface, and its mathematical form is:

$$\Delta p = \gamma\left(\frac{1}{R_1} + \frac{1}{R_2}\right) \tag{2}$$

Δp is pressure difference between interface surfaces, γ is surface tension, R_1 and R_2 are major radii of interface curvature. For oil-water separation process, the effect of separation can be directly affected by the change of interface curvature.

(3) Capillary force equation

The capillary force is an important factor that influences oil-water separation rate. In accordance with the principle of capillary action, the capillary force can be calculated as follows:

$$F_c = \gamma \cdot \cos\theta \cdot L \tag{3}$$

Among them, F_c is the capillary force, γ is the surface tension. The capillary force has a close relationship with the wettability of graphene surface during the separation process. By adjusting graphene's surface properties, capillary force can be controlled effectively.

(4) Relationship between surface wettability and separation efficiency

The hydrophobicity of graphene has a significant effect on oil/water separation efficiency. The contact angle can be used to describe the wettability of graphene, and the relation between the contact angle θ and the separation efficiency can be expressed as:

$$E = A \cdot \cos\theta \tag{4}$$

E is the separation efficiency, and A is a constant. Through the adjustment of the contact angle, it is possible to optimize the oil and water separation efficiency.

(5) Kinetic model of oil-water separation

Oil and water separation process not only depends on the physical parameters, but also on the separation dynamics. The kinetic behavior of the separation process can be described by the following equation:

$$\frac{dC}{dt} = -k \cdot C \tag{5}$$

Among them, C is the oil concentration in the oil-water mixture, and k is the separation rate constant. This equation shows that oil-water separation is a time-varying process, and the oil concentration will gradually decrease as the separation process proceeds.

(6) Effect of temperature on oil-water separation

Temperature plays an important role in oil and water separation efficiency. Changes in temperature affect liquid viscosity and surface tension, thus affecting separation efficiency [10]. The relationship between temperature and separation efficiency can be expressed as:

$$E(T) = E_0 \cdot \exp\left(-\frac{Q}{RT}\right) \tag{6}$$

$E(T)$ is the separation efficiency at temperature T, E_0 is a constant, Q is the activation energy, and R is the gas constant. This formula explains the effect of temperature on oil-water separation. Generally, an increase in temperature will increase the separation efficiency.

(7) Effect of surface modification on separation efficiency

Temperature plays an important role in oil and water separation efficiency. The change of temperature affects liquid viscosity and surface tension, so it is effective for improving the separation efficiency of graphene. It is possible to modify the graphene surface by changing its hydrophilicity or hydrophobicity. It was found that the modified graphene material had better separation properties [11]. The relationship between separation efficiency and graphene surface energy after surface modification is expressed as follows: efficiency. The relationship between temperature and separation efficiency can be expressed as:

$$E_{\text{mod}} = E_0 \cdot \left(1 + \frac{S_{\text{new}}}{S_{\text{old}}}\right) \tag{7}$$

Among them, E_{mod} is the separation efficiency after surface modification, S_{new} and S_{old} are the surface energies after and before modification, respectively.

(8) Comprehensive separation efficiency model

In practical applications, the comprehensive efficiency of graphene oil-water separation is not only related to factors such as surface properties, capillary action, and interfacial tension, but also affected by a variety of factors. The comprehensive separation efficiency model can be expressed by the following formula:

$$E_{\text{total}} = f(E_1, E_2, E_3, \cdots, E_n) \tag{8}$$

Among them, $E_1, E_2, E_3, \cdots, E_n$ represent the contribution of different factors to the separation efficiency. This model can provide guidance for the optimization of graphene oil-water separation process.

3. Design and implementation of computer simulation system

3.1. System architecture design

The design goal of this system is to achieve efficient and accurate numerical simulation and provide intuitive result visualization to help users understand and optimize the separation process. The architecture of the simulation system consists of three major modules: preprocessing, solving and postprocessing.

The main function of the pre-processing module is to generate the geometric structure and meshing of the simulation model. In order to ensure the calculation accuracy, the graphene oil-water separation system needs to be finely modeled during the simulation process. In this module, users can create a computational model by inputting experimental conditions (such as the physical properties of the fluid, the characteristics of the graphene surface, etc.). The physical domain needs to be meshed and the mesh needs to be refined to capture complex phenomena such as the oil-water interface and capillary action. The pre-processing module is also responsible for generating initial conditions and boundary conditions for the subsequent solution module.

The solution module is the key part of the simulation system, which is responsible for solving the mathematical model. In this system, FEA and CFD are applied to the numerical calculation of graphene oil and water separation. Through the solution of Navier-Stokes equation, Young Laplacian equation, capillary force equation and so on, the paper can get the parameters of fluid flow, interface change, separation efficiency and so on. Because of the large amount of computation involved, this module requires high computational power and optimized algorithms.

The post-processing module is responsible for extracting the calculation results from the solution module and visually displaying them. This module not only provides the display of numerical results, such as oil-water separation efficiency, flow rate, pressure distribution, etc., but also can display the simulation results in the form of images, curves, animations, etc. through a graphical interface, which is convenient for users to analyze and understand. Users can adjust the simulation conditions through the interactive interface and observe the effects of different parameters on the separation process.

3.2. Selection of numerical methods

The choice of numerical method directly influences the precision and computing efficiency of the simulation system. For the complicated flow and interface problems of graphene oil-water separation, the usual numerical methods are FEA and FDM. Each has its own merits and demerits, and the concrete selection depends on the features and requirements of the problem. The finite element method is widely applied in the field of engineering, especially for the analysis of complicated geometry structures. The FEA method can be applied to solve the complicated problems of fluid dynamics, capillary action and interface tension. The FEA method can deal with complicated boundary and nonlinear problems, and can be used to describe the variation of fluid and interface in water separation. The finite difference method is a kind of simple numerical method, which can be used to solve relatively simple geometry model and linear problem. Under certain conditions, FDM can be combined with the FEM to calculate the flow velocity and pressure field in the oil-water separation process.

4. Experiment and simulation

4.1. Experimental platform construction

In order to conduct graphene oil-water separation experiments, a suitable experimental platform needs to be built in a laboratory environment. The platform can not only simulate the actual oil-water separation process, but also provide accurate experimental data for comparison with computer simulation results.

The core equipment of the experimental platform includes oil-water separation device, flow meter, pressure sensor, temperature sensor and data acquisition system. The oil-water separation device consists of a graphene-coated filter membrane, a collection tank, a fluid delivery system, and other parts. The flow meter is used to accurately measure the flow rate of the input fluid, the pressure sensor is used to monitor the pressure change during the separation process, and the temperature sensor is used to control and record the temperature during the experiment. The data acquisition system collects the data of the above sensors in real time, and processes and stores them. The preparation method of graphene materials directly affects the performance of oil-water separation. On the experimental platform, chemical vapor deposition (CVD) is used to prepare graphene membranes with excellent hydrophilicity and oleophobicity. Parameters such as the porosity, surface characteristics, and membrane thickness of the graphene membrane can be controlled by adjusting the CVD process conditions, thereby affecting the efficiency and stability of oil-water separation. The experiment first requires the graphene membrane to be installed in the separation device, and the flow rate, temperature, pressure and other parameters of the liquid are adjusted. The oil-water mixture enters the separation device through the fluid delivery system and flows through the graphene membrane for separation. By controlling different operating conditions, the pressure changes, separation efficiency, stability and other indicators during the separation process are recorded.

4.2. Experimental Design

In order to comprehensively evaluate the performance of graphene oil-water separation, the experimental design needs to consider a variety of influencing factors, including flow rate, temperature, pressure, and surface properties of graphene membranes. When designing the experiment, the following aspects are focused on:

Different oil-water ratios may affect the separation efficiency of graphene membranes. Therefore, the experiment first designs experimental schemes with different oil-water ratios to test the separation effect of graphene membranes under different oil-water ratios. The results of these experiments may be helpful for the determination of the effect of oil/water ratio on the separation properties of graphene. The flow rate is the main factor that influences the separation process, and the higher the flow rate, the lower the separation efficiency. Through the experiment, the flow rate of liquid is adjusted to test the effect of separation. Furthermore, the relation of the flow velocity and the pore size of the graphene membrane must be taken into account, and the optimal flow control strategy can be obtained. Temperature and pressure also affect the separation properties of graphene membranes significantly. Higher temperatures may change the surface properties of graphene membranes, thus affecting the affinity of oil and water; while pressure affects the speed of liquid flow and interfacial tension. In the experiment, the influence of temperature and pressure on the separation properties of graphene was evaluated. The surface properties of graphene films, including contact angle, surface roughness, film thickness, etc. have a direct influence on the performance of oil and water separation. In this paper, the influence of the surface treatment method of graphene film on the separation efficiency was investigated.

Moreover, it is possible to adjust the flow rate to match the surface characteristics of graphene film to obtain optimal separation efficiency. It is difficult for the oil/water mixture to pass effectively through the membrane at a lower flow rate, and at higher flow rates, the separation performance of the membrane can be reduced. Thus, the optimum flow rate can increase the separation efficiency and prolong the lifetime of graphene film. Through the optimization of the surface characteristics, such as contact angle and surface roughness, it is possible to increase the hydrophilicity or oleophobicity of the film, thus improving the efficiency of oil and water separation. The simulation system is used to simulate graphene membranes with different surface properties, predict their separation effects under different conditions, and provide a theoretical basis for the experiment. The long-term stability of the graphene oil-water separation system is also one of the key goals of optimization. By simulating the performance changes of graphene membranes during long-term use through simulation systems, theoretical support can be provided for the maintenance and replacement cycle of the membranes, and the use strategy of the separation system can be optimized.

5. Results and Discussion

Oil and water mixture is separated by graphene film in the simulation. In order to get a better understanding of the fluid flow on the membrane surface, a simulation system is developed to simulate the flow field at various flow rates and operating conditions. Figure 1 illustrates the distribution of the flow field at various flow rates. When the flow rate is increased, the fluid's kinetic energy is increased, which leads to a more even flow of fluid over the membrane. The flow of the fluid presents a greater vortex effect at a lower flow rate and a poor separation effect; at a higher flow rate, the fluid flow is more stable and can be more efficiently separated through the graphene film.

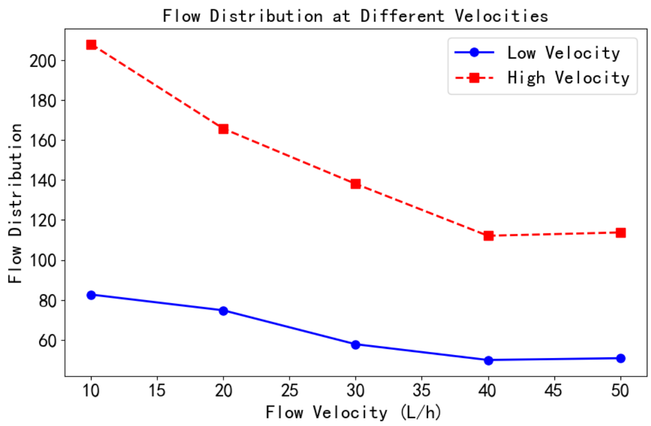

Figure 1. Flow field distribution at different flow rates

The oil-water separation process of graphene membrane is affected by interfacial tension, and the interface morphology is crucial to the separation efficiency. Figure 2 shows the morphology of the oil-water interface under different operating conditions. The results in Figure 2 show that the interfacial tension changes significantly with the change of operating pressure and temperature. Higher operating pressure helps to reduce the interfacial tension, thereby improving the effect of oil-water separation. Under a certain pressure, the separation of the oil-water interface is more obvious, indicating that the graphene membrane has good hydrophilic and oleophobic properties.

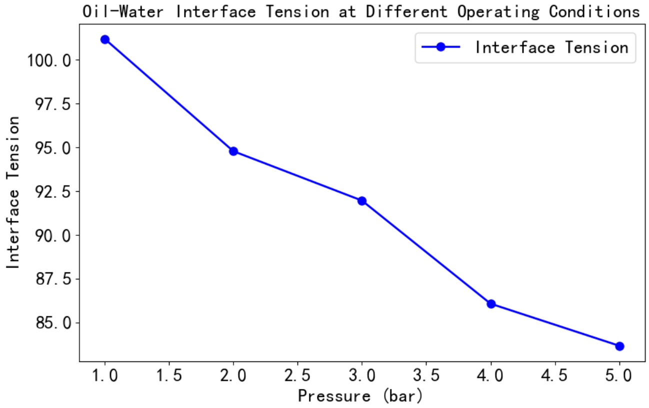

Figure 2. Oil-water interface morphology under different operating conditions

In order to verify the accuracy of the simulation model, this paper compares the experimental results with the simulation results. Table 1 shows the separation efficiency data obtained from the experiment and simulation under different flow rates and oil-water ratios. The results of the experiment and the simulated results are very similar, and there are little errors, which shows that the model can predict well. In particular, at a lower flow rate and a 2: 1 ratio of oil and water, the error is within 1%. The results indicate that the model can be used to predict the separation efficiency of graphene oil and water separation.

Table 1. Comparison of experimental and simulation results

Flow rate (L/h)	Oil-water ratio	Experimental separation efficiency (%)	Simulated separation efficiency (%)	Error (%)
10	1:01	89.5	88.7	0.9
20	1:01	85.3	86.1	0.8
10	2:01	91.2	90.5	0.7
20	2:01	87.8	88	0.2

Although the simulation model is very close to the experimental results, small errors can still be observed in some cases. These errors may come from several factors: there are certain measurement errors in the experiment, such as the control accuracy of flow rate and pressure, which may affect the accuracy of the results. In the simulation, this paper makes simplified assumptions on some physical processes, such as ignoring the influence of dissolved gas, which may cause the simulation results under certain special conditions to deviate from the experimental data.

Separation efficiency is the core indicator in the graphene oil-water separation process. According to the experimental and simulation results, this paper can evaluate the separation efficiency under different conditions. Table 2 shows the separation efficiency data under different oil-water ratios. With the increase of oil-water ratio, the separation efficiency of graphene membrane increases. Especially when the oil-water ratio is 3:1, the separation efficiency is close to 92%, which shows that the graphene membrane has good performance for the separation of high oil ratio.

Table 2. Separation efficiency at different oil-water ratios

Oil-water ratio	Separation efficiency (experimental)	Separation efficiency (simulation)
1:01	89.50%	88.70%
2:01	91.20%	90.50%
3:01	92.40%	92.00%

Flux is another important indicator for evaluating the performance of separation membranes. A high flux means that the graphene membrane can process more oil-water mixture per unit time. Figure 3 shows the separation flux under different flow rate conditions. As the flow rate increases, the separation flux increases significantly. This is because a higher flow rate allows the oil-water mixture to pass through the graphene membrane faster, thereby increasing the separation flux. However, too high a flow rate may cause clogging of the membrane, so a trade-off needs to be made between flow rate and separation efficiency.

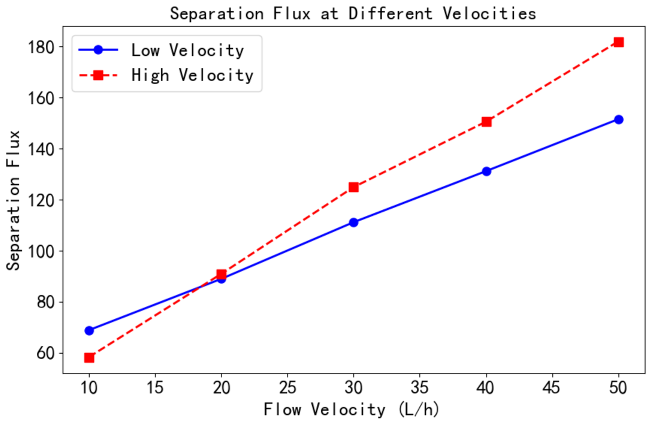

Figure 3. Separation flux at different flow rates

The stability of the graphene oil-water separation membrane is an important indicator to measure its long-term performance. In order to evaluate the stability of the membrane, this paper conducted a long-term experiment and recorded the changes in the separation efficiency and flux of the membrane over time. Figure 4 shows the changes in the separation efficiency of the graphene membrane at different usage times. The graphene membrane showed a high separation efficiency during the initial use, and the separation efficiency decreased slightly with the increase in usage time. After 72 hours of use, the separation efficiency of the membrane remained at about 90%, indicating that the graphene membrane has good long-term stability, but further optimization is still needed to improve its anti-fouling ability.

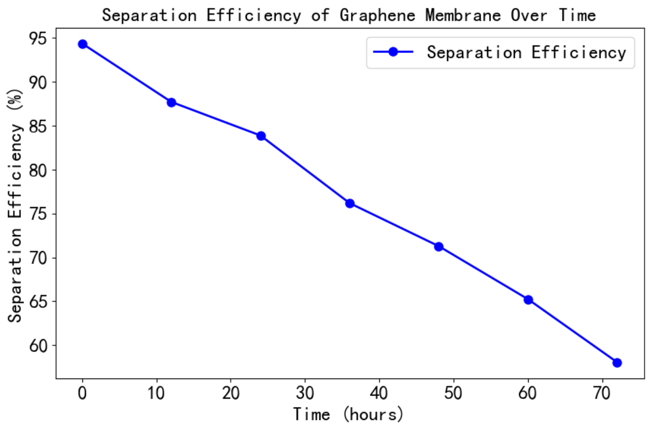

Figure 4. Changes in separation efficiency of graphene membranes at different usage times

6. Conclusion

The deep learning-based graphene oil-water separation process simulation and computer simulation technology application system proposed in this paper successfully achieved accurate prediction and optimization of the graphene oil-water separation process. By establishing physical and mathematical models, a simulation platform based on FEA and CFD was designed, and experimental verification was carried out to prove the application value of the system in graphene oil-water separation technology. However, there are still some limitations in the current research. First, the scale of the experimental data set is relatively small, and future research should expand the sample size to cover more types of graphene materials to improve the generalization ability of the model. Secondly, the real-time performance and stability of the intelligent monitoring system still need to be further improved to meet the high requirements in practical applications.

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