Numerical simulation of oil droplets spreading on solid surface in water

Zhiwen Chen, Xiaoyong Yang, Bingjie Wang, Jian Dai, Zhishan Bai*

School of Mechanical and Power Engineering, East China University of Science and Technology, Shanghai, 200237, China

*Corresponding author’s e-mail: baizs@ecust.edu.cn

Abstract. Plate separators are widely used for oil-water separation in the petrochemical industry. The spreading process of oil droplets at the solid surface is the key to understanding the oil-water separation mechanism in the plate separator. This study uses VOF method to capture oil-water phase interface change and sets up a two-dimensional model of oil droplets spreading on solid surface in water. The influences of droplet diameter, oil-water interfacial tension and viscosity are studied. The numerical simulation results show that the maximum spreading length of oil droplets increases with the increase of droplet size and interfacial tension. The average spreading speed of oil droplets decreases with the increase of oil droplet size, and increases with the increase of surface tension. The maximum spreading length and average spreading speed of oil droplets decrease with the increase of the dynamic viscosity of the oil droplets.

1. Introduction
Oily wastewater generated in the production process of petrochemical industry is one of the important sources of water pollution[1]. Plate separator integrates gravitational settling, shallow pool theory and coalescence technology, which is widely used in the field of oil-water separation due to the advantages of no consumption of chemicals, easy maintenance, low operating cost and no secondary pollution[2]. The spreading process of oil droplets at the solid surface is the key to understanding the oil-water separation mechanism in the plate separator. With the development of computer technology, computer numerical simulation calculation are more and more widely used in scientific research. Sun et al.[3] used the coupling model of VOF and level set to simulate the morphological change characteristics of the droplet after impacting the superhydrophobic wall, and found that the impact process can be divided into four stages: drop, expansion, contraction, and rebound. Li et al.[4] used the VOF method to calculate the impact force during the process of the droplet impacting on the solid wall, and found that the maximum impact force occurred on both sides of the center of droplet during the spreading process. Gunjal et al.[5] explored the influence of droplet size, viscosity and velocity on the droplet spreading radius, and established the model of a single droplet impacting the wall.

However, numerical simulation studies of the spreading process of liquid droplets on solid walls are mostly in the gas phase environment, and the size of the droplets are all millimeter level. This paper investigates the spreading process of micron oil droplets on solid walls in a liquid environment. This study sets up a two-dimensional model of oil droplets spreading on solid surface in water, and the VOF model is used to investigate the influence of oil droplet diameter, oil-water interfacial tension and viscosity on the spreading process of oil droplets on solid walls.
2. Model and methods

2.1. VOF model

The VOF method is one of the commonly used methods in multiphase flow interface tracking methods. This method realizes the simulation of the flow between two or more immiscible fluids by solving a single momentum equation and the volume fraction of the fluid passing through the region.

Where the fluid volume fraction $\alpha_k$ in the unit cell is expressed as:

$$
\alpha_k(x,y,z,t) = \begin{cases} 
1 & \text{Phase } k \text{ is filled} \\
0 & \text{Phase } k \text{ is not contained} \\
0 \sim 1 & \text{Phase interface}
\end{cases}
$$

(1)

In each cell:

$$
\sum_k \alpha_k = 1
$$

(2)

Solving the continuity equation of the phase volume ratio, $\alpha_k$ can be obtained:

$$
\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = 0
$$

(3)

where $\rho_k$ is the density of the $k$ phase fluid, $\mathbf{u}_k$ is the velocity vector of the $k$ phase fluid.

2.2. Numerical method

![Figure 1](image1.png)

Figure 1. (a) Two-dimensional geometric model; (b) mesh division.

The two-dimensional geometric model shown in Figure 1(a) is established. The size of the geometric model is $5 \text{ mm} \times 2 \text{ mm}$, the initial particle size of the oil droplet is $D$, and the initial velocity is $\mathbf{u}$. Using this geometric model for numerical simulation calculations, the following assumptions were made during the simulation process: the shape of the oil droplet is spherical before it impacts the solid wall; the distance between the droplet and the solid wall at the initial moment is $0.01D$; the wall is assumed to be absolutely smooth; the contact Angle is assumed to be constant during spreading.

The near-wall grid is encrypted by using ICEM, where the smallest grid thickness is $2 \mu\text{m}$, as shown in Figure 1(b). The structured staggered grid containing 225000 cells is used for numerical simulations. The upper boundary is set as a non-slip wall, and the surrounding boundary is set as a
pressure inlet. CSF (Continuous surface force) model and geometric reconstruction model are used to construct the phase interface. The pressure-based implicit splitting of operators (PISO) algorithm is used to consider a coupling between the velocity and pressure terms. In the beginning of a simulation, a spherical drop was patched in the computational domain (volume fraction of oil phase was set to 1) with an impact velocity in vertically upwards direction (at time $t=0$). The discretized form of the prescribed equations is solved by using flow solver Fluent.

$d$ is defined as the spreading length, and $d/D$ is defined as the dimensionless spreading length. The specific simulation parameter settings are shown in Table 1.

### Table 1. Parameter settings in numerical simulation.

| Parameter                        | Unit       | Continuous phase (water) | Discrete phase (isooctane) |
|----------------------------------|------------|---------------------------|----------------------------|
| Density                          | kg/m$^3$   | 998                       | 687                        |
| Viscosity                        | mPa*s      | 0.895                     | 0.479                      |
| Surface tension                  | mN/m       | 0.072                     | 0.021                      |
| Oil-water interfacial tension    | mN/m       |                           | 0.047                      |
| Initial diameter of oil droplet  | μm         |                           | 810                        |
| Impact velocity                  | m/s        |                           | 0.041                      |
| Contact angle                    | °          |                           | 85                         |

#### 2.3. Model validation

In order to verify the accuracy of the model, this study experimentally investigated the spreading process of isooctane oil droplets with a diameter of 810 μm and an impact velocity of 0.041 m/s on a...
solid wall with a wettability of 85°. The experimental results are compared with the simulation results. Figures 2 and 3 show the comparison of the experimental and numerical simulation results of the morphological changes of oil droplets and the dimensionless spread length during the spreading process. It can be seen that the experimental value of oil droplet morphology change is in good agreement with the simulated value, and the simulated value of dimensionless spreading length is larger than the experimental value. The maximum dimensionless spreading length of the simulated and experimental values are 1.72 and 1.55 respectively. The numerical simulation results show that the oil droplets shrink back when it reach the maximum spread length on the solid wall surface. The error between the experimental value and the simulated value is about 10% during the spreading stage. The error is caused by the fact that the solid wall is simplified into an absolutely smooth wall without roughness and the contact angle is considered to be constant during the spreading process. Although there are errors in the model, the comparison results between the simulated and experimental values of the changes in droplet morphology and dimensionless spreading length from wetting to maximum spreading are all within acceptable range. Therefore, the feasibility of this model is verified to simulate the spreading process of oil droplets on solid wall surface.

3. Results and discussion

3.1. Droplet size

Figure 4 shows the changes in the spreading process of oil droplets with diameters of 1800 μm, 1300 μm, 800 μm and 300 μm impacting the solid wall at the same speed of 0.041m/s, and the static contact angle is 85°. For oil droplets with diameters of 300 μm, 800 μm, 1300 μm and 1800 μm, it can be seen that the maximum dimensionless spreading lengths are 1.68, 1.72, 1.79 and 1.88, respectively. The time to reach the maximum spreading length is 1.5ms, 6.5ms, 12.5ms and 19.5ms, respectively. The average speed of spreading was 0.34m/s, 0.21m/s, 0.19m/s and 0.17m/s. With the increase of droplet size, the average spreading speed of oil droplet decreases, while the spreading time and maximum dimensionless spreading length increase. Under the condition of the same impact velocity, with the increase of the particle size of oil droplets, the kinetic energy before impact also increases, which leads to the increase of the maximum spreading length.

3.2. Oil-water interfacial tension

Figure 5 shows the dimensionless spreading length of oil droplets spreading on the solid wall with the diameter of 800 μm, an impact velocity of 0.041m/s, the static contact angle of 85° and a interfacial tension of 0.02 N/m, 0.05 N/m, 0.08 N/m and 0.14 N/m, respectively. It can be seen that the time to
reach the maximum spread length is 9.5 ms, 6.25 ms, 4 ms and 3 ms respectively, and the maximum dimensionless spreading length is 1.72, 1.72, 1.79 and 1.89 respectively. The average spreading speed is 0.14m/s, 0.22m/s, 0.36m/s and 0.5m/s respectively. With the increase of oil-water interfacial tension, the droplet spreading speed is faster, and the spreading time is shorter, and the maximum dimensionless spreading length is larger. Under the same impact kinetic energy condition, the conversion rate between free surface energy and kinetic energy is faster with the increase of surface tension. Therefore, the droplet spreads faster and takes less time with the increase of surface tension.

![Figure 5. Effect of interfacial tension on spreading](image)

3.3. Viscosity

Figure 6 shows the dimensionless spreading length of oil droplets spreading on the solid wall with the diameter of 800 μm, an impact velocity of 0.041m/s, the static contact angle of 85° and a dynamic viscosity of 0.1 mPa·s, 0.5 mPa·s, 1.5 mPa·s and 10 mPa·s, respectively. It can be seen that the maximum dimensionless spreading length is 1.80, 1.74, 1.66, 1.55 and 1.46 respectively. The time to reach the maximum spreading length is 6.25ms, 6.5ms, 6.75ms, 7.75ms and 8.5ms, respectively. The average spreading speed is 0.23m/s, 0.21m/s, 0.20m/s, 0.16m/s and 0.14m/s. With the increase of the dynamic viscosity of oil droplets, more energy is dissipated by the viscous force inside the oil droplets during the spreading process. Therefore, the average spreading speed and the maximum spreading

![Figure 6. Effect of viscosity on spreading.](image)
length decrease successively. The propagation of capillary waves in the spreading process of oil droplets with a viscosity of 10 mPa·s is slower and stable compared with the Oil droplet with a viscosity of 0.1 mPa·s. As the viscosity of the oil droplet increases, the frictional resistance between its internal molecules increases, and the attenuation speed of the capillary wave propagation on its surface increases, resulting in the deformation process to be slower.

4. Conclusion
The VOF model is used in this study. Based on the numerical simulation method, the effect of oil droplet physical properties on the spreading process is investigated. The results show that the maximum spreading length of oil droplets increases with the increase of droplet size and interfacial tension. However, the maximum spreading length and average spreading velocity of oil drop decrease with the increase of dynamic viscosity of oil droplets phase.

Acknowledgements
This work was support by the National Natural Science Foundation of China, China (22078102), the Scientific Research Projects of Shanghai, China (19DZ1208201) and China Postdoctoral Science Foundation (2019TQ0094).

References
[1] J K Joshi, S D Bhattacharya, S Maiti, I M Mishra, Removal of oil from oil-in-water emulsion using a packed bed of commercial resin[J]. Colloids and Surfaces, A. Physicochemical and Engineering Aspects 2011, 389: 291-298.
[2] Y Han, L He, X Luo, Y Lü, K Shi, J Chen, X Huang, A review of the recent advances in design of corrugated plate packs applied for oil–water separation[J]. Journal of Industrial and Engineering Chemistry 2017, 53.
[3] J Sun, Q Liu, Y Liang, Z Lin, C Liu. Biological Design and Manufacturing 2019, 2: 10-23.
[4] R Li, H Ninokata, M Mori, A numerical study of impact force caused by liquid droplet impingement onto a rigid wall[J]. Progress in Nuclear Energy 2011, 53.
[5] P R Gunjal, V V Ranade, R V Chaudhari, Dynamics of drop impact on solid surface: Experiments and VOF simulations[J]. Aiche Journal 2005, 51.