

1. Building 2D Models

The calculation area is set to be 6 mm×6 mm, where the solid area is 1 mm×6 mm and the watershed is 5 mm×6 mm. Set the width of the notch to be a , the depth of the square column to be h , and the width of the square column to be b .

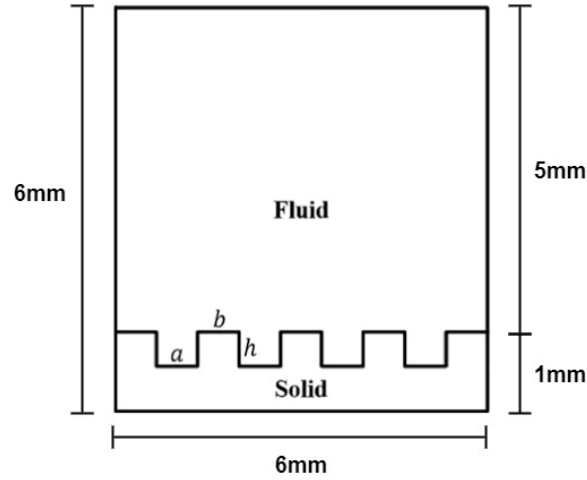


Figure S1 Schematic of the 2D model

Set a to 25 μm , h to 20 μm , b to 10、25、50、75 μm .

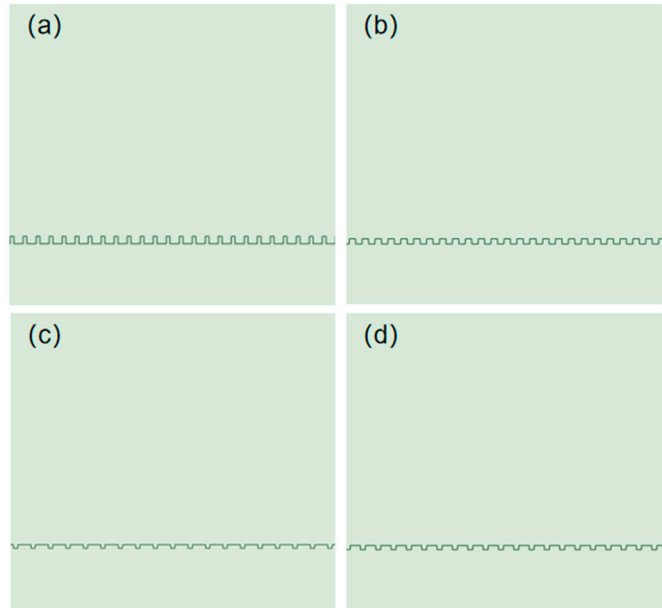


Figure S2 (a)The 2D model when b is 10 μm ; (b)The 2D model when b is 25 μm ;

(c)The 2D model when b is 75 μm ; (d)The 2D model when b is 50 μm

2. Meshing

The element size of the mesh is set to 0.1 mm and the CFD method is selected for meshing, the solver preference is selected as Fluent and the element order is selected as Linear.

Display		Quality	
Display Style	Use Geometry Setting	Check Mesh Quality	Yes, Errors
Defaults		<input type="checkbox"/> Target Skewness	Default (0.900000)
Physics Preference	CFD	Smoothing	Medium
Solver Preference	Fluent	Mesh Metric	None
Element Order	Linear	Inflation	
<input type="checkbox"/> Element Size	0.1 mm	Use Automatic Inflat...	None
Export Format	Standard	Inflation Option	Smooth Transition
Export Preview Surfa...	No	<input type="checkbox"/> Transition Ratio	0.272
Sizing		<input type="checkbox"/> Maximum Layers	2
Use Adaptive Sizing	No	<input type="checkbox"/> Growth Rate	1.2
<input type="checkbox"/> Growth Rate	Default (1.2)	Inflation Algorithm	Pre
Mesh Defeaturing	Yes	View Advanced Opti...	No
<input type="checkbox"/> Defeature Size	Default (5.e-004 mm)	Batch Connections	
Capture Curvature	Yes	Mesh Based Connec...	No
<input type="checkbox"/> Curvature Min Si...	Default (1.e-003 mm)	Advanced	
<input type="checkbox"/> Curvature Norm...	Default (18.0°)	Number of CPUs for ...	Program Controlled
Capture Proximity	No	Straight Sided Eleme...	
Size Formulation (Be...	Program Controlled	Rigid Body Behavior	Dimensionally Redu...
Bounding Box Diag...	84.853 mm	Triangle Surface Me...	Program Controlled
Average Surface Area	1800.0 mm²	Use Asymmetric Ma...	No
Minimum Edge Len...	5.e-002 mm	Topology Checking	Yes
Enable Size Field (Be...	No	Use Sheet Thickness ...	No
		Pinch Tolerance	Default (9.e-004 mm)
		Generate Pinch on R...	No
		Sheet Loop Removal	No
		Statistics	
		<input type="checkbox"/> Nodes	368489
		<input type="checkbox"/> Elements	367382

Figure S3 Parameter Settings for Meshing

3.Models and parameterize

Set the direction of gravity to the negative direction of the y-axis with a magnitude of -9.8m/s^2 .

General

Mesh

Scale... Check Report Quality

Display... Units...

Solver

Type

☒ Pressure-Based

☐ Density-Based

Velocity Formulation

☒ Absolute

☐ Relative

Time

☐ Steady

☒ Transient

2D Space

☒ Planar

☐ Axisymmetric

☐ Axisymmetric Swirl

☐ Adjust Solver Defaults Based on Setup

☒ Gravity

Gravitational Acceleration

X (m/s²) 0

Y (m/s²) -9.8

Z (m/s²) 0

Figure S4 Gravity settings

The VOF model is selected for the simulation. Implicit body force is used in the

simulation.

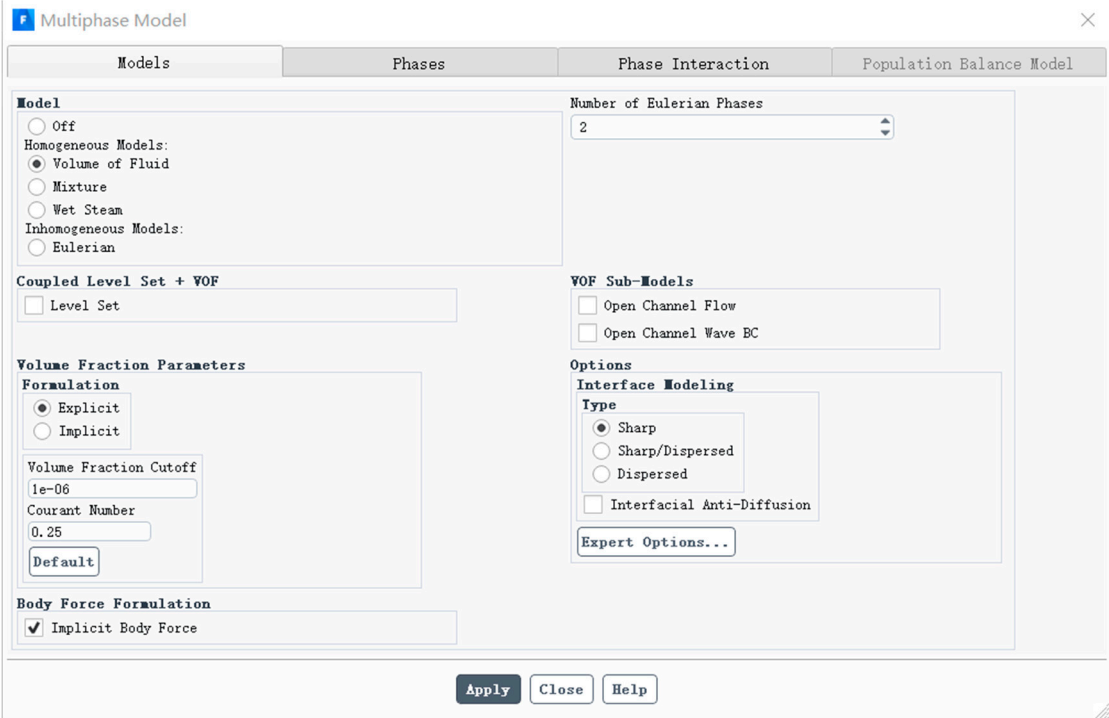


Figure S5 Model Settings

Set phase 1 to be air and phase 2 to be water.

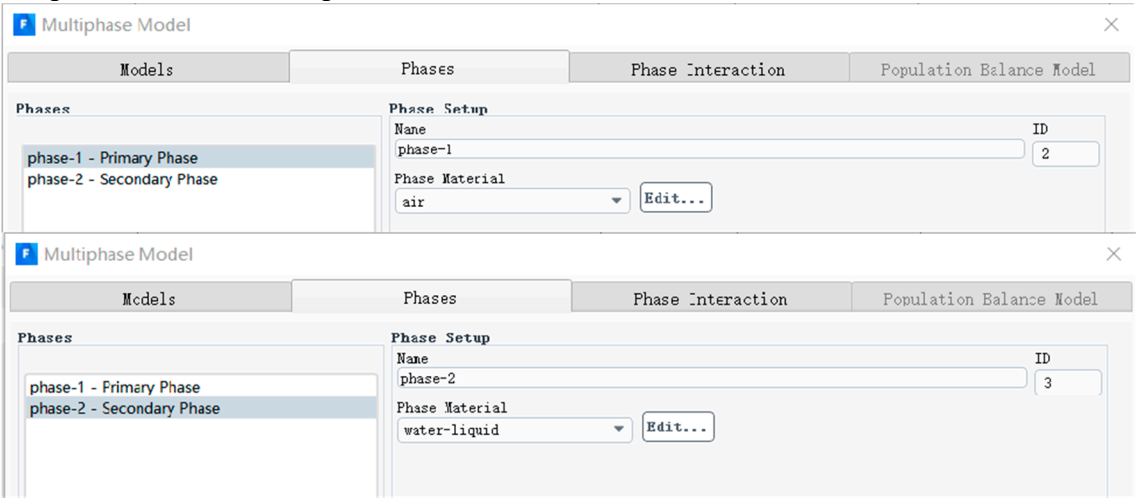


Figure S6 Phase settings

Set the density of air to 1.225 kg/m³, the viscosity of air to 1.789×10⁻⁵ kg/(m·s) and the density of water to 998 kg/m³, the viscosity of water to 0.001 kg/(m·s).

The screenshot shows the 'Create/Edit Materials' dialog box for a material named 'air'. The 'Name' field contains 'air'. The 'Material Type' is set to 'fluid'. The 'Chemical Formula' field is empty. The 'Fluent Fluid Materials' dropdown is set to 'air'. The 'Mixture' dropdown is set to 'none'. The 'Order Materials by' section has 'Name' selected. The 'Properties' section shows 'Density (kg/m3)' set to 'constant' with a value of 1.225, and 'Viscosity (kg/m-s)' set to 'constant' with a value of 1.7894e-05. At the bottom are buttons for 'Change/Create', 'Delete', 'Close', and 'Help'.

Field	Value
Name	air
Material Type	fluid
Chemical Formula	
Fluent Fluid Materials	air
Mixture	none
Density (kg/m3)	constant, 1.225
Viscosity (kg/m-s)	constant, 1.7894e-05

Figure S7 The parameter settings of the air

The screenshot shows the 'Create/Edit Materials' dialog box for a material named 'water-liquid'. The 'Name' field contains 'water-liquid'. The 'Material Type' is set to 'fluid'. The 'Chemical Formula' field contains 'h2o<1>'. The 'Fluent Fluid Materials' dropdown is set to 'water-liquid (h2o<1>)'. The 'Mixture' dropdown is set to 'none'. The 'Order Materials by' section has 'Name' selected. The 'Properties' section shows 'Density (kg/m3)' set to 'constant' with a value of 998.2, and 'Viscosity (kg/m-s)' set to 'constant' with a value of 0.001003. At the bottom are buttons for 'Change/Create', 'Delete', 'Close', and 'Help'.

Field	Value
Name	water-liquid
Material Type	fluid
Chemical Formula	h2o<1>
Fluent Fluid Materials	water-liquid (h2o<1>)
Mixture	none
Density (kg/m3)	constant, 998.2
Viscosity (kg/m-s)	constant, 0.001003

Figure S8 The parameter settings of the water

The surface tension coefficient between water and air is 0.073 N/m. Considering the effect of surface tension, surface tension force modelling is chosen and the model is selected as Continuum Surface Force and the Adhesion Options is selected as Wall Adhesion.

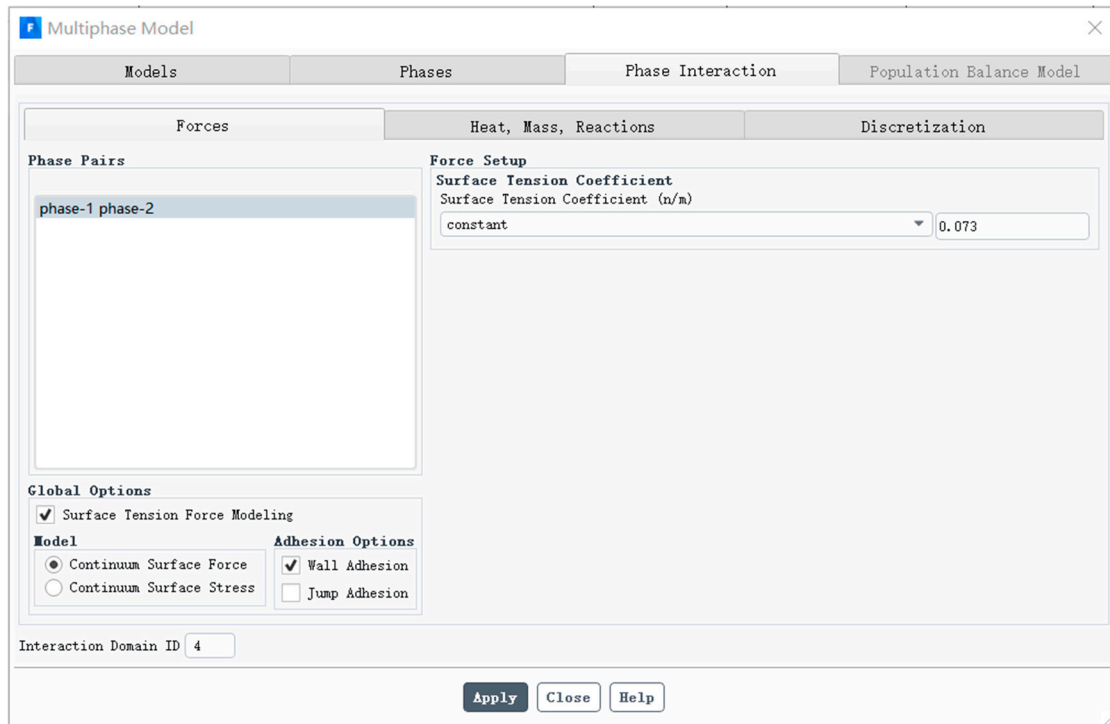


Figure S9 The settings of the phase interaction
Set the viscous model to Laminar.

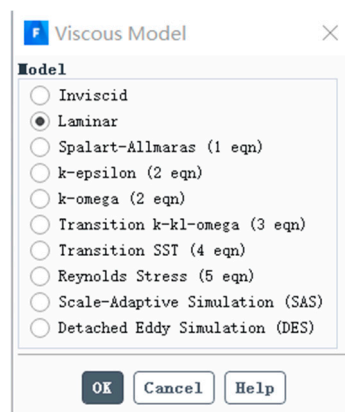


Figure S10 The settings of the viscous model
The solid material was selected as PTFE and its density was set to be 2450 kg/m³.

Create/Edit Materials

Name: Material Type: Order Materials by: ☒ Name ☐ Chemical Formula

Chemical Formula: Fluent Solid Materials:

Mixture:

Properties

Density (kg/m3):

Figure S11 The parameter settings of the solid material
Set the solid material surface as a stationary No Slip Wall.

Wall

Zone Name: Phase:

Adjacent Cell Zone: Shadow Face Zone:

Momentum Thermal Radiation Species DPM Multiphase UDS Potential Structure

Wall Motion **Motion**

☒ Stationary Wall ☐ Moving Wall ☒ Relative to Adjacent Cell Zone

Shear Condition

☒ No Slip ☐ Specified Shear ☐ Specularity Coefficient ☐ Marangoni Stress

Wall Roughness

Roughness Height (nm): Roughness Constant:

Wall Adhesion

Contact Angles (deg):

Figure S12 The settings of the solid material surface
The upper, left and right boundaries of the fluid are set as pressure outlet boundary.

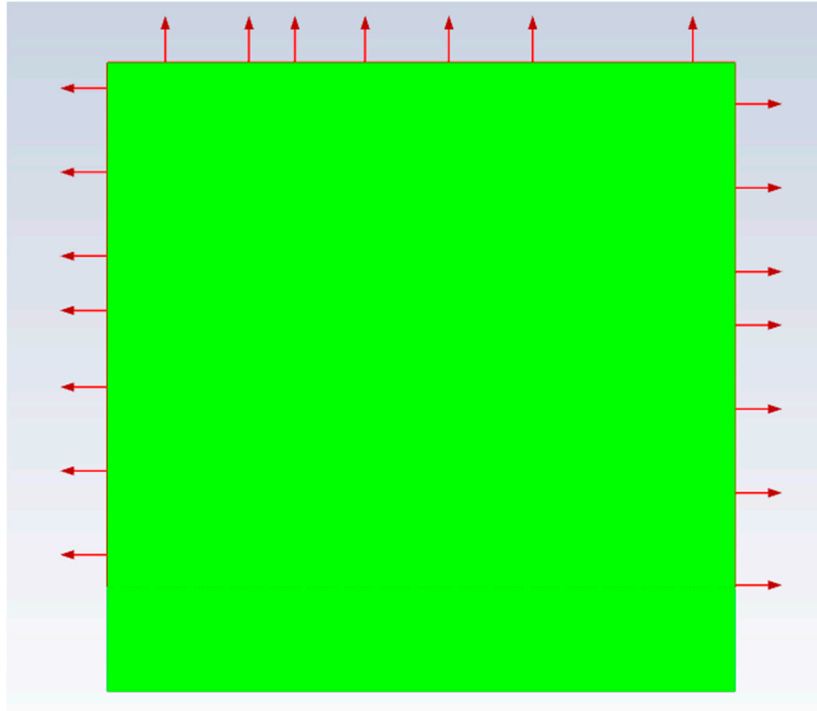


Figure S13 The settings of the pressure outlet boundary

Draw a unit register in the fluid, initialized as a water droplet, which has a diameter of 2 mm and is initially located at a tangent to the top of the square column.

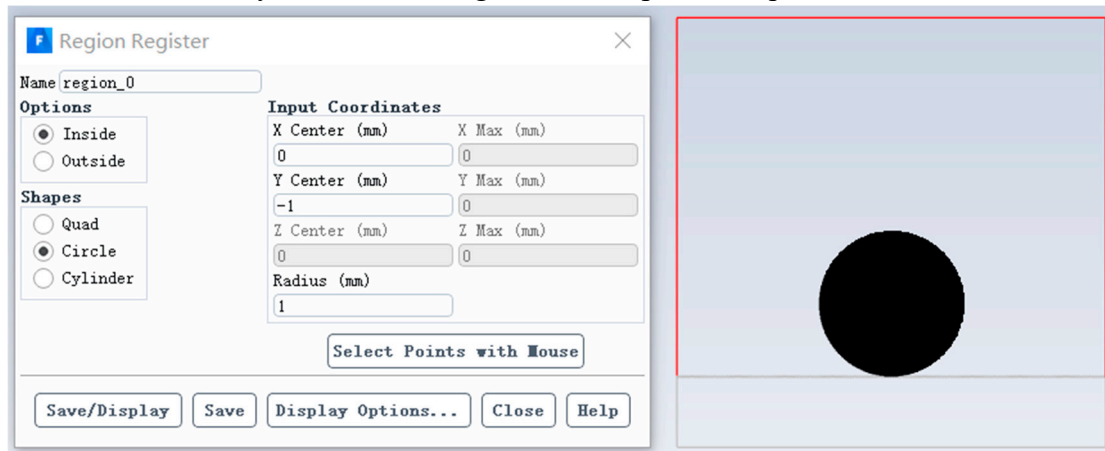


Figure S14 The settings of the droplet

The scheme is set as PISO algorithm. The gradient is Least Squares Cell Based, the pressure is Body Force Weighted, the volume fraction is Geo-Reconstruct, and the momentum is Second Order Upwind.

Solution Methods ?

Pressure-Velocity Coupling

Scheme: PISO

Skewness Correction: 1

Neighbor Correction: 1

☒ Skewness-Neighbor Coupling

Spatial Discretization

Gradient: Least Squares Cell Based

Pressure: Body Force Weighted

Momentum: Second Order Upwind

Volume Fraction: Geo-Reconstruct

Transient Formulation

First Order Implicit

☐ Non-Iterative Time Advancement

☐ Frozen Flux Formulation

☐ Warped-Face Gradient Correction

☐ High Order Term Relaxation Options...

☐ Reduced Rank Extrapolation Options...

Default

Figure S15 The settings of the solution methods

During initialization, the velocity of the droplet in both the x and y directions is set to 0, and the gauge pressure and the volume fraction are also set to 0.

Solution Initialization ?

Initialization Methods

☐ Hybrid Initialization

☒ Standard Initialization

Compute from: ▼

Reference Frame

☒ Relative to Cell Zone

☐ Absolute

Initial Values

Gauge Pressure (pascal): 0

X Velocity (m/s): 0

Y Velocity (m/s): 0

phase-2 Volume Fraction: 0

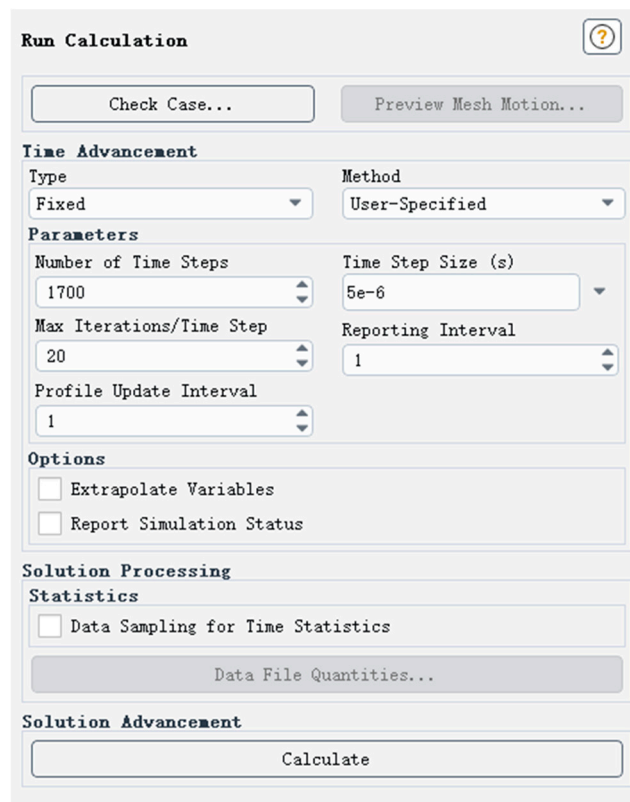
Initialize Reset Patch...

Reset DPM Sources Reset LWF Reset Statistics

VOF Check

Figure S16 The settings of the solution initialization

The calculation values were set up to simulate the gradual stabilization of a water droplet on a surface over 10 ms by setting the time step size to 5e-6s, the number of time steps to 1700 and the max iteration/time step to 20.



The 'Run Calculation' dialog box contains the following settings:

- Buttons:** 'Check Case...' and 'Preview Mesh Motion...'.
- Time Advancement:**
 - Type: Fixed
 - Method: User-Specified
- Parameters:**
 - Number of Time Steps: 1700
 - Time Step Size (s): 5e-6
 - Max Iterations/Time Step: 20
 - Reporting Interval: 1
 - Profile Update Interval: 1
- Options:**
 - ☐ Extrapolate Variables
 - ☐ Report Simulation Status
- Solution Processing:**
 - Statistics: ☐ Data Sampling for Time Statistics
 - Data File Quantities...
- Solution Advancement:**
 - Calculate

Figure S17 The settings of the calculation

Simulation Result

The steady state of the water droplets on each rough structure was obtained at the simulation's end and is shown in Fig S18.

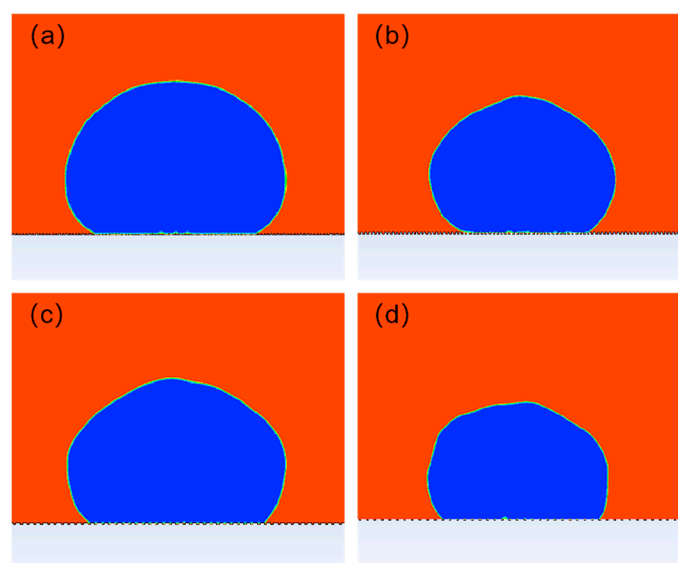


Figure S18. (a) Water droplet steady state at T value of 5:2; (b) Water droplet steady state at T value of 1:1; (c) Water droplet steady state at T value of 1:2; (d) Water droplet steady state at T value of 1:3

After obtaining the corresponding results, they were imported into Photoshop for graphic processing to enhance the droplet contours and facilitate identification by the Engauge Digitizer, as shown in Fig S19.

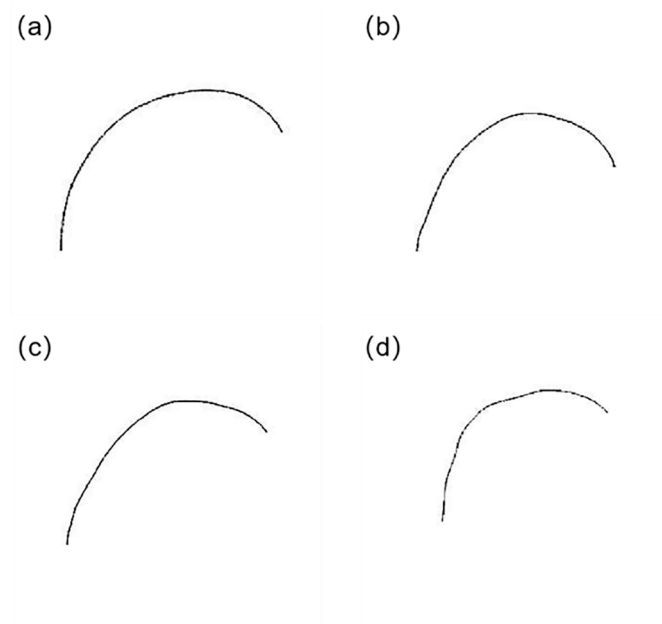


Figure S19. (a) Profile at T value of 5:2; (b) Profile at T value of 1:1; (c) Profile at T value of 1:2; (d) Profile at T Value 1:3

The processed image is then imported into the Engauge Digitizer, where the aspect ratio determines the coordinate values of the three reference points, from which the values of the other coordinates on the contour line are calculated, as shown in Figure S20.

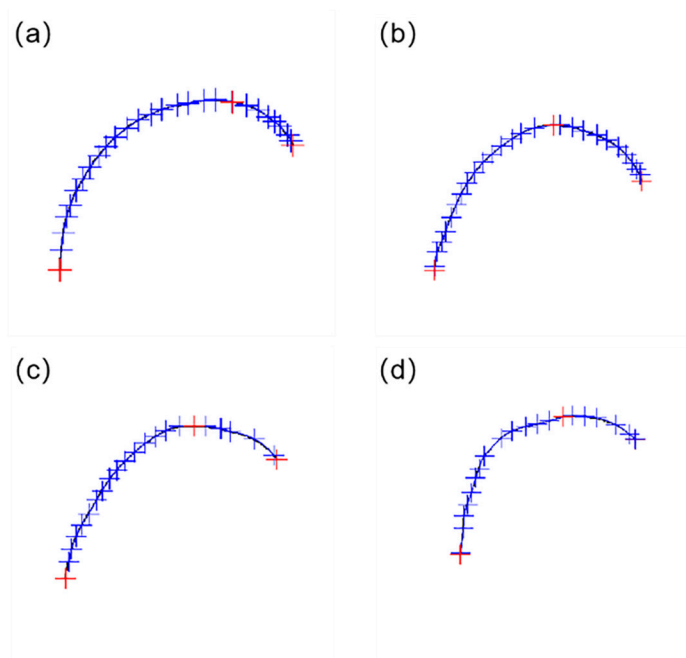


Figure S20. (a) Fitting points at T value of 5:2; (b) Fitting points at T value of 1:1; (c) Fitting points at T value of 1:2; (d) Fitting points at T value of 1:3

The coordinate values obtained from the fitting process were imported into MATLAB for curve-appropriate purposes. Each curve's equation was derived, and its corresponding value

was obtained. The contour curve fits exhibited a high level of accuracy, with a fitting accuracy of 99 percent, indicating a robust, appropriate effect. The equations of the fitted curves is shown in Figure S21.

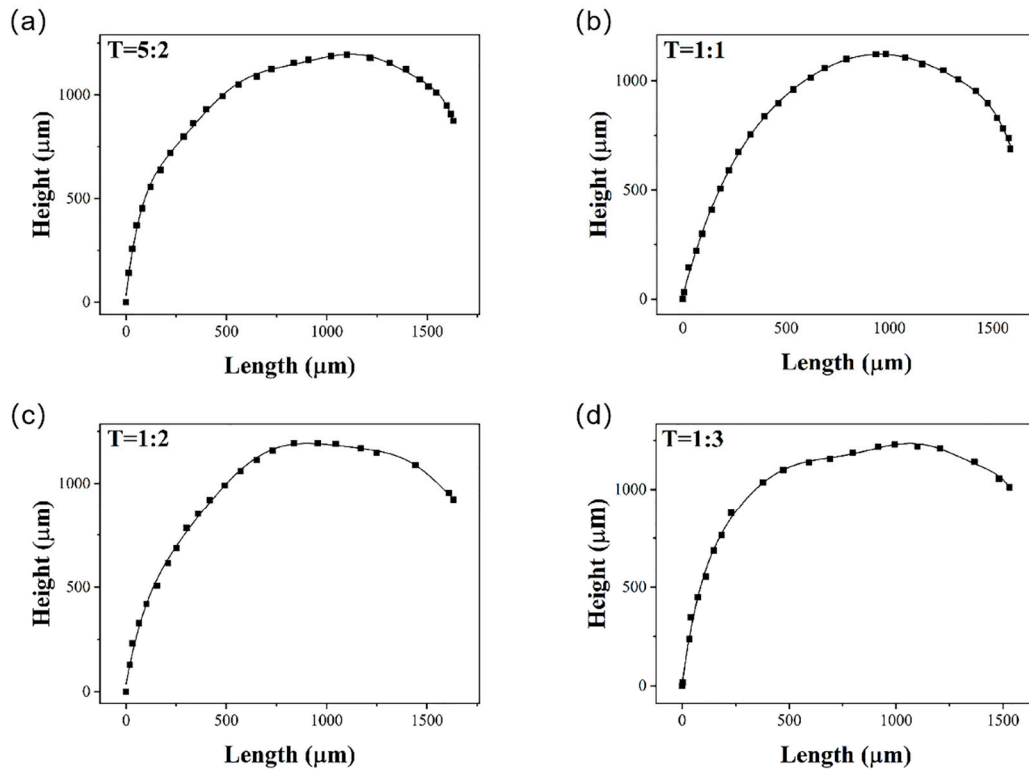


Figure S21. (a) curve of the fitted function at T value of 5:2; (b) curve of the fitted function at T value of 1:1; (c) curve of the fitted function at T value of 1:2; (d) curve of the fitted function at T value of 1:3

$T = 5:2$:

$$f(x) = -1.189 \times 10^{-20} x^8 + 8.176 \times 10^{-17} x^7 - 2.323 \times 10^{-13} x^6 + 3.52 \times 10^{-10} x^5 - 3.07 \times 10^{-7} x^4 + 1.556 \times 10^{-4} x^3 - 4.509 \times 10^{-2} x^2 + 8.06x + 34.04 \quad (S1)$$

$T = 1:1$:

$$f(x) = -1.237 \times 10^{-20} x^8 + 6.171 \times 10^{-17} x^7 - 1.223 \times 10^{-13} x^6 + 1.302 \times 10^{-10} x^5 - 9.852 \times 10^{-7} x^4 + 7.381 \times 10^{-4} x^3 - 5.712 \times 10^{-2} x^2 + 3.557x + 17.8 \quad (S2)$$

$T = 1:2$:

$$f(x) = 1.538 \times 10^{-18} x^7 - 1.092 \times 10^{-14} x^6 + 3.062 \times 10^{-11} x^5 - 4.363 \times 10^{-8} x^4 + 3.397 \times 10^{-5} x^3 - 1.54 \times 10^{-2} x^2 + 4.973x + 43.75 \quad (S3)$$

$T = 1:3$:

$$f(x) = -1.375 \times 10^{-20} x^8 + 8.756 \times 10^{-17} x^7 - 2.294 \times 10^{-13} x^6 + 3.199 \times 10^{-10} x^5 - 2.587 \times 10^{-7} x^4 + 1.259 \times 10^{-4} x^3 - 3.859 \times 10^{-2} x^2 + 8.279x + 9.257 \quad (S4)$$

The contact angles for each microstructure surface were determined as follows: 165.9°, 160.4°, 146.4°, and 146° based on the derived results.

The dimensions of these four structures are then utilized in the following equation for calculation. The calculated results are subsequently compared with the simulation results to validate the accuracy of the simulation.

$$f_s = \frac{b}{a+b} \quad (S5)$$

$$f_s + f_a = 1 \quad (S6)$$

$$\cos \theta = \frac{b^2 \cos \theta_s - a^2 - 2ab}{(a+b)^2} \quad (S7)$$

The simulation results and calculations corresponding to each value are shown in the table below.

Table S1. Simulation results and calculation results corresponding to each T value

T	1:3	1:2	1:1	5:2
Simulation				
Results	146°	146.4°	160.4°	165.9°
Calculation				
Results	132°	137.4°	148.4°	162.1°
Error Value	9.6%	6.1%	7.5%	2.3%
f_s	0.75	0.67	0.5	0.29

The discrepancies between the simulation and calculated results are all below 10 percent, as presented in the table above. Therefore, we can conclude that the simulation results are basically consistent with the calculated results

As the ratio of the width of the groove to the width of the square column increases, several effects are observed:

- 1、The contact area of the water droplets on the solid-liquid contact surface, relative to the projected area of the solid-liquid contact surface, decreases.
- 2、The contact angle of the water droplets on the solid surface increases.
- 3、The hydrophobicity of the solid surface is significantly enhanced.