Recent Advances in Droplet and Spray Simulations

In Celebration of Prof. Wen-Hann Sheu's 60th Birthday

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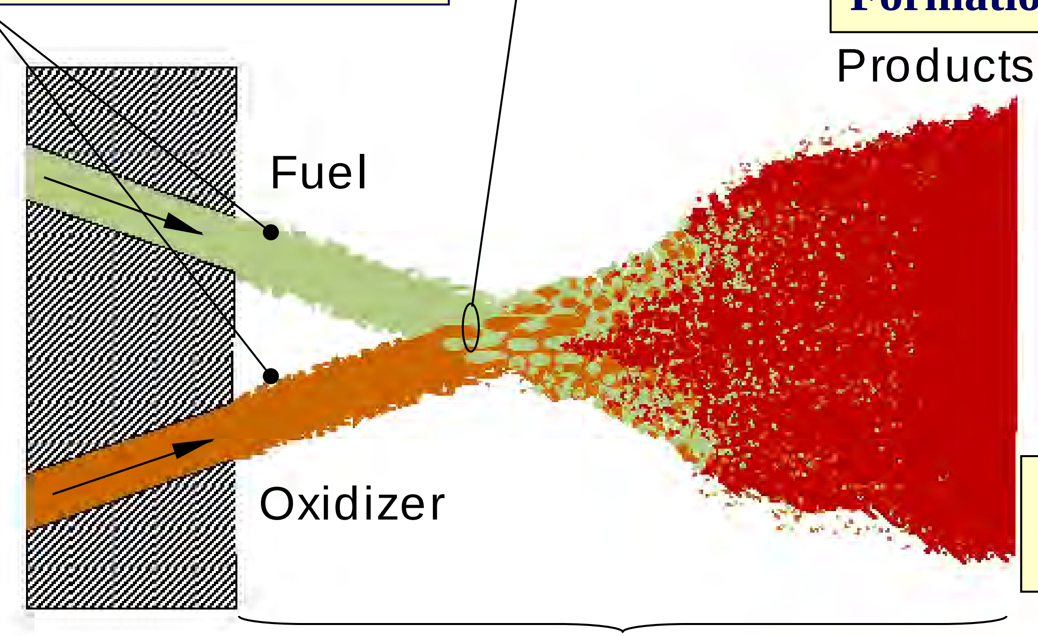
Impinging Jets

3. Interfacial Reactions and Transport at Atomistic, Molecular, Micro, and Meso Scales

1. Materials Formulation, Processing, and Characterization

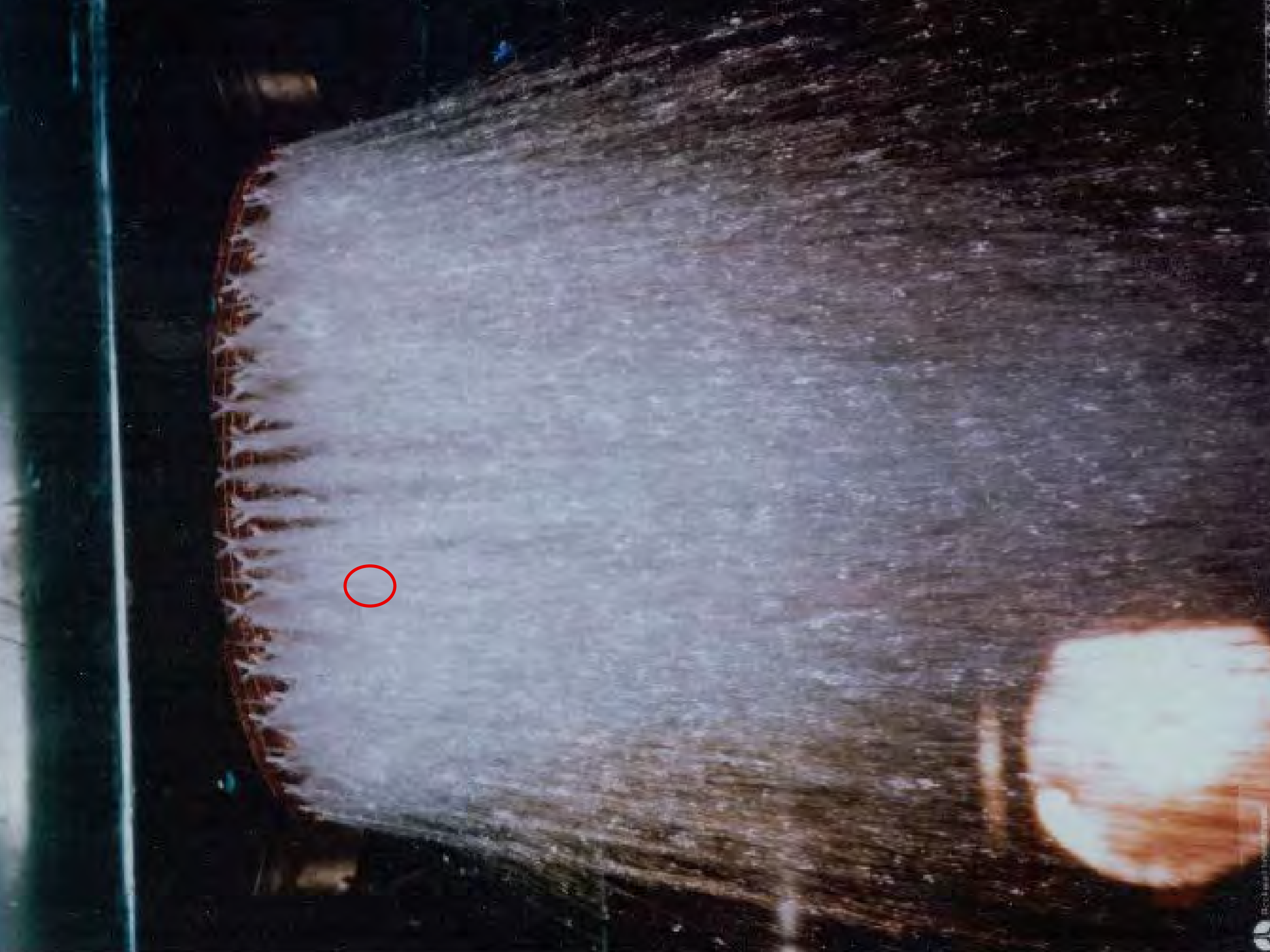
2. Jet Atomization, Spray Formation, and Droplet Dynamics



4. Ignition and Reaction Mechanisms in Gas Phase

5. Modeling, Simulation, and Diagnostics of Overall Processes

Yang, GaTech



Governing Equations

- **Incompressible, variable-density, Navier-Stokes equations:**

$$\rho(\partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}) = -\nabla p + \nabla\cdot(2\mu\boldsymbol{D}) + \sigma\kappa\delta_s\boldsymbol{n}$$

$$\partial_t\rho + \nabla\cdot(\rho\boldsymbol{u}) = 0$$

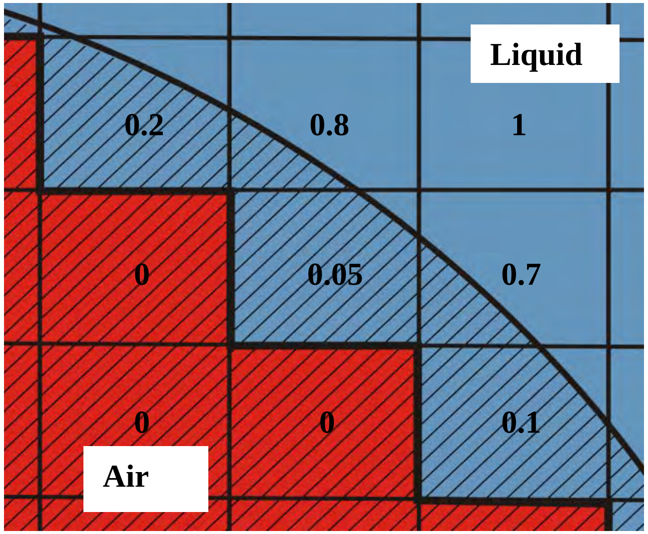
$$\nabla\cdot\boldsymbol{u} = 0$$

- **Volume fraction, two-phase fluid density and viscosity:**

$$\rho(c) \equiv c\rho_1 + (1-c)\rho_2,$$
$$\mu(c) \equiv c\mu_1 + (1-c)\mu_2,$$

- **Advection for volume fraction:**

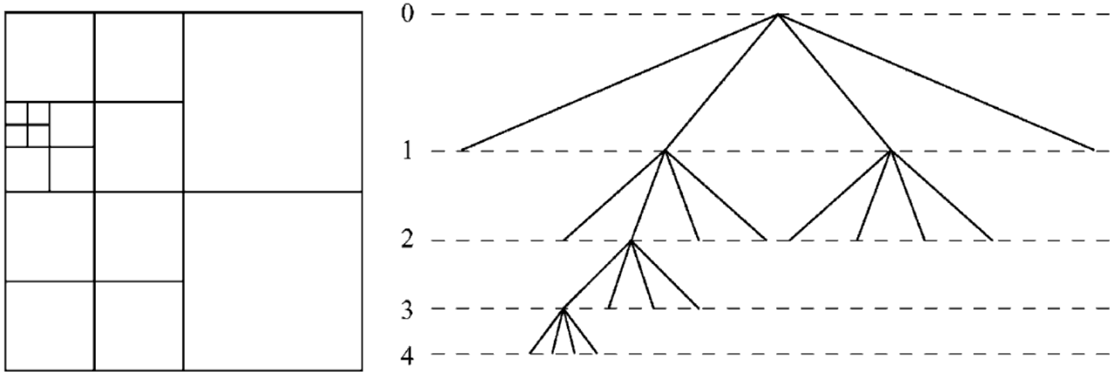
$$\partial_t c + \nabla\cdot(c\boldsymbol{u}) = 0$$

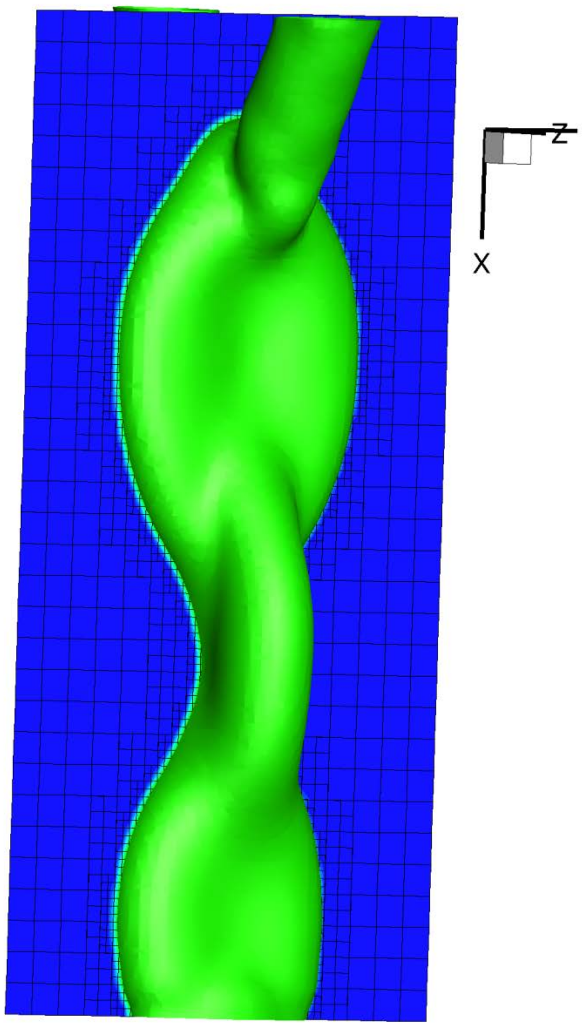


Coupled Eulerian Volume-of-Fluid and Lagrangian Particle Tracking Method

- **Coupling between Eulerian/Lagrangian algorithms:**
  - Two-way coupling approach is implemented for the interaction between Eulerian flow field and Lagrangian particles;
  - Smooth force distribution is used to resolve different size particles.
- **Conversion of small droplets from Eulerian description into Lagrangian particles:**
  - Eulerian droplets smaller than a prescribed threshold volume are removed (void fraction set to zero) and replaced by a Lagrangian point particle;
  - Lagrangian point particles can be transformed back into a VOF-resolved droplet based on its proximity with the VOF interface or pre-specified region;
  - Other criterions such as droplet sphericity are being tested;
  - The transformations have been integrated into the AMR framework.

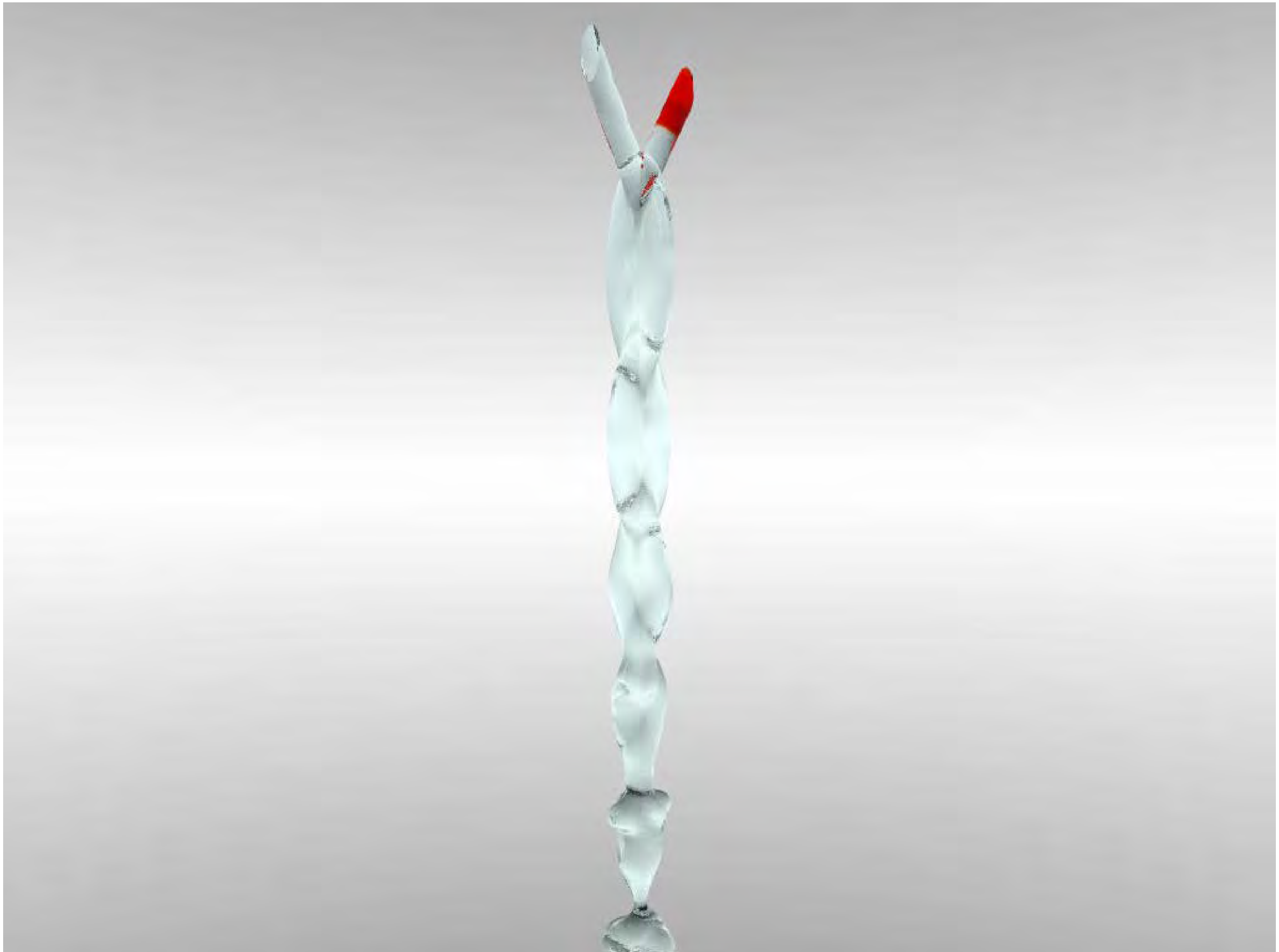
Adaptive Mesh Refinement





- **Quad/Octree AMR Gerris code by Popinet S. (J. Comput. Phys. 2003, 2009);**
- **Improve interfacial resolution and computational efficiency;**
- **Efficient to deal with reconnection and breakup of interfaces;**
- **Refinement criteria: voticity, gradient, curvature etc.**

We=27.5, Re=1000, D=0.5 mm, U=2 m/s, ρ=1000 kg/m^3, μ= 1$\times$10^{-3} N·s/m^2



Breakup Regimes and Mechanisms

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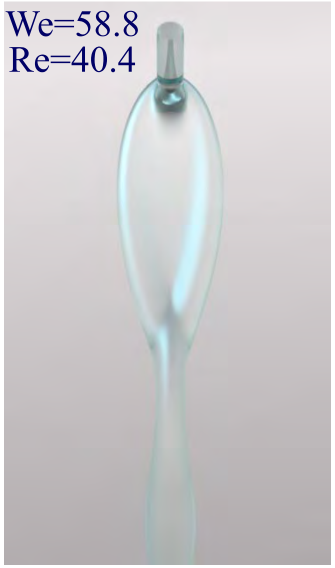
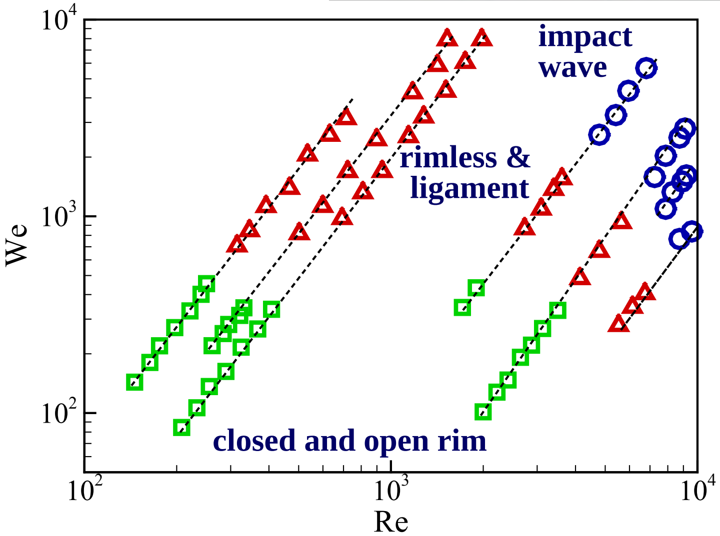


- Characteristic parameters:

  $$\mathrm{Re}=\rho DU/\mu,\ \ \mathrm{We}=\rho DU^2/\sigma,$$

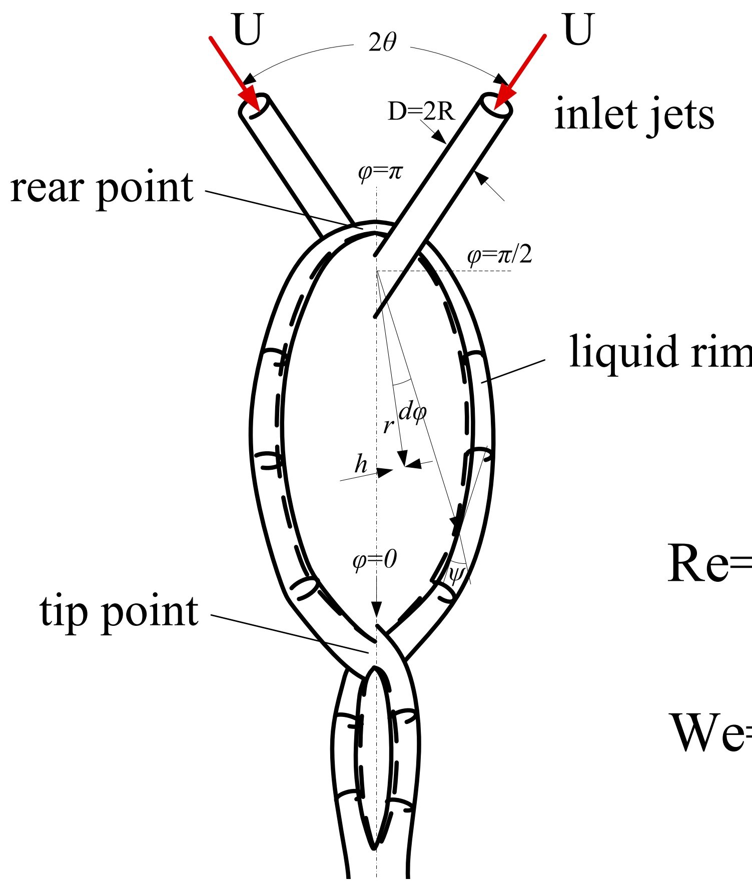
  $$\mathrm{Oh}=\mu\Big/\sqrt{\rho D\sigma}=\sqrt{\mathrm{We}}\Big/\mathrm{Re}$$

- Capillary instability (low speed)
- Kelvin-Helmholtz instability (medium speed)
- Impact wave mechanism (high speed)



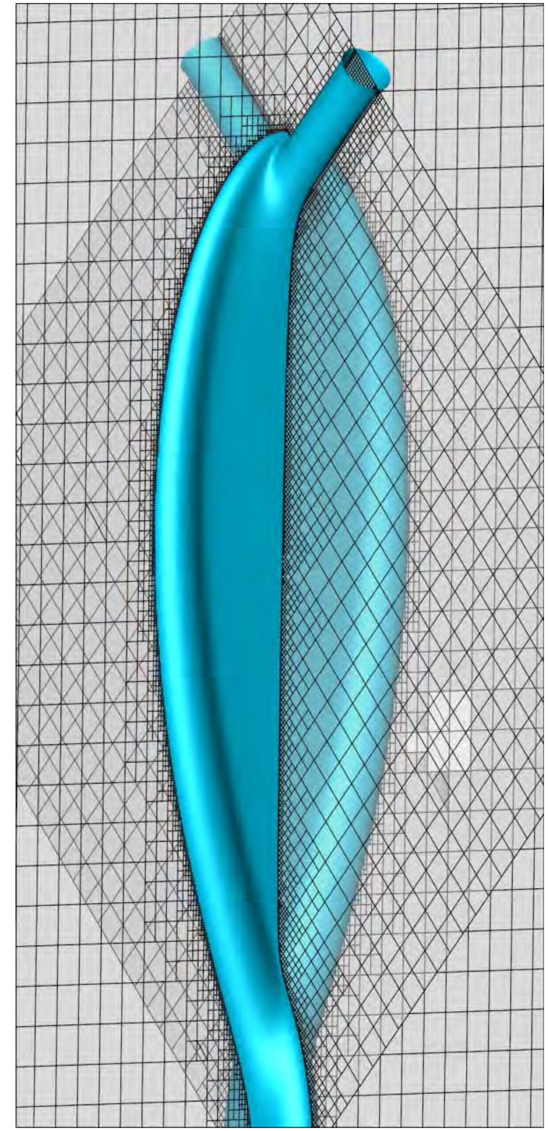
Regime diagram produced by H. K. Ciezki et al. 2006

Verfication of Low-Velocity Impinging Jets



$$\mathrm{Re} = \frac{\rho D U}{\mu}$$

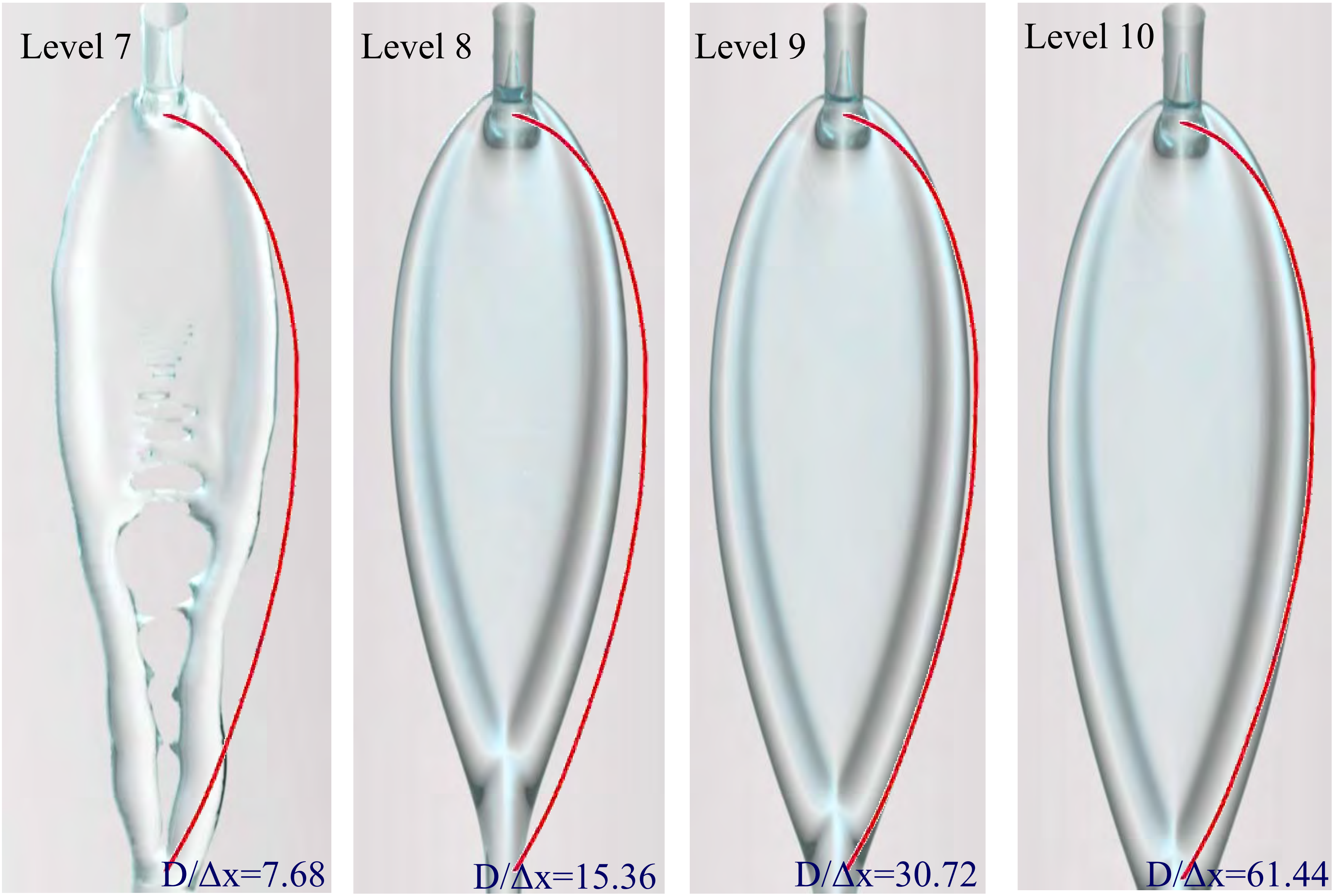
$$\mathrm{We} = \frac{\rho D U^2}{\sigma}$$



ρ_{liq} kg/m^3	ρ_{air} kg/m^3	μ_{liq} kg/m/s	μ_{air} kg/m/s	σ N/m	Re	We
998	1.29	0.001	0.000001	0.076	40.4	58.8

Rim Pattern Under Different Grid Resolution

Glycerine–Water Jets, D_j = 0.4 mm, V_j = 6 m/s, 2θ = 90º, Re = 40.4, We = 58.8



Atomization Under Different Grid Resolution

Water Jets, D_j = 0.635 mm, V_j = 18.5 m/s, 2θ = 60º, Re = 11724, We = 2987

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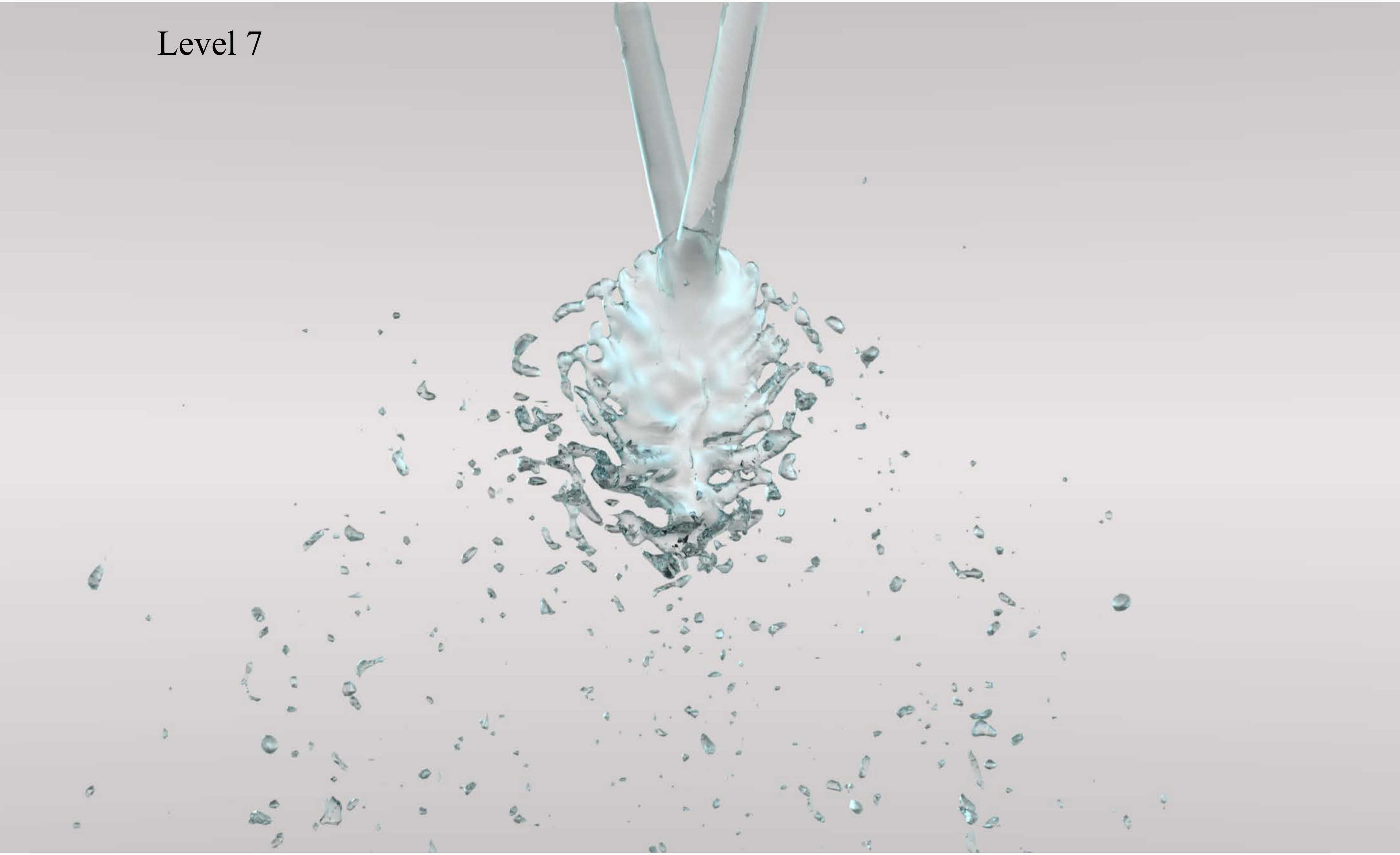
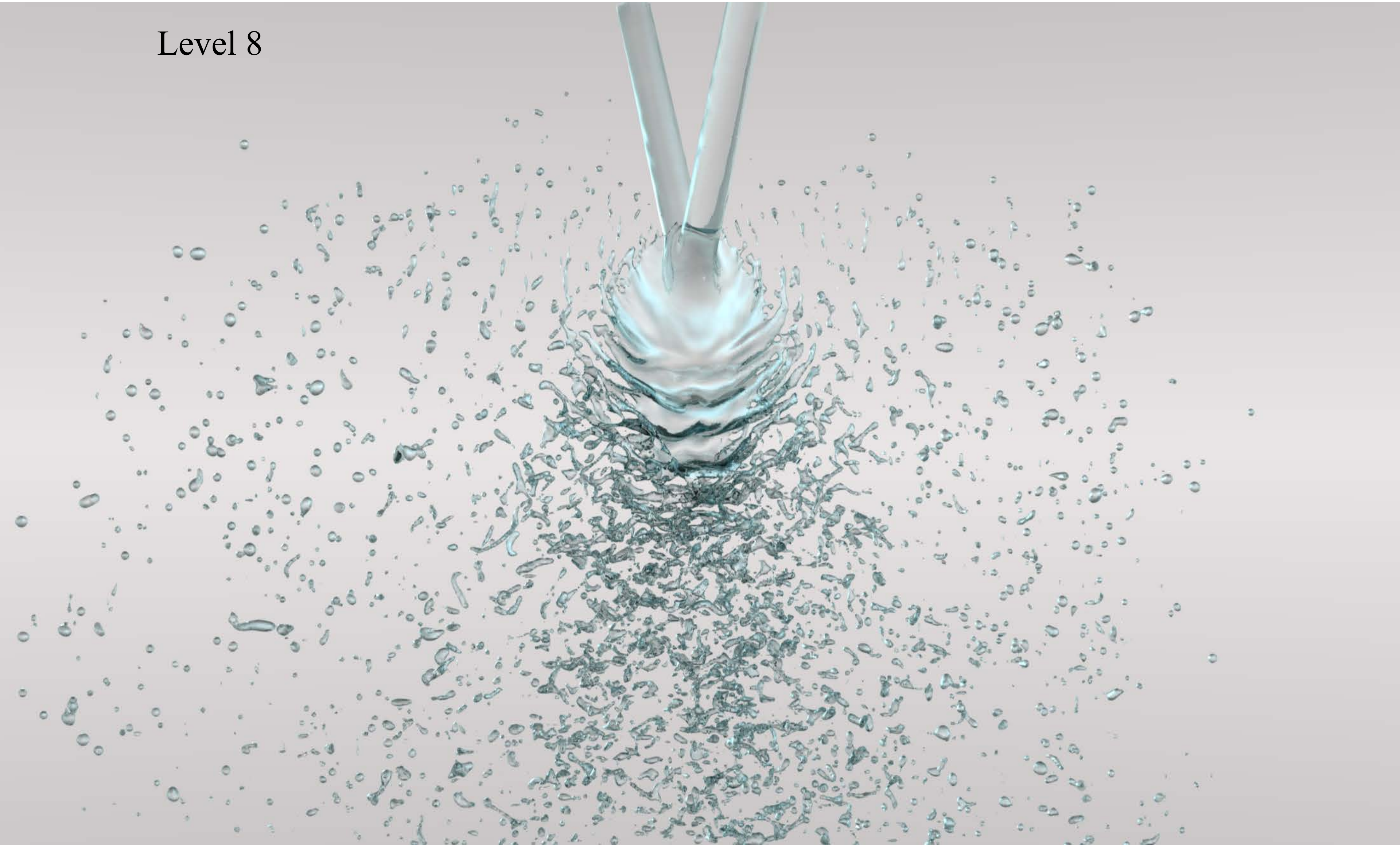


Atomization Under Different Grid Resolution



Atomization Under Different Grid Resolution

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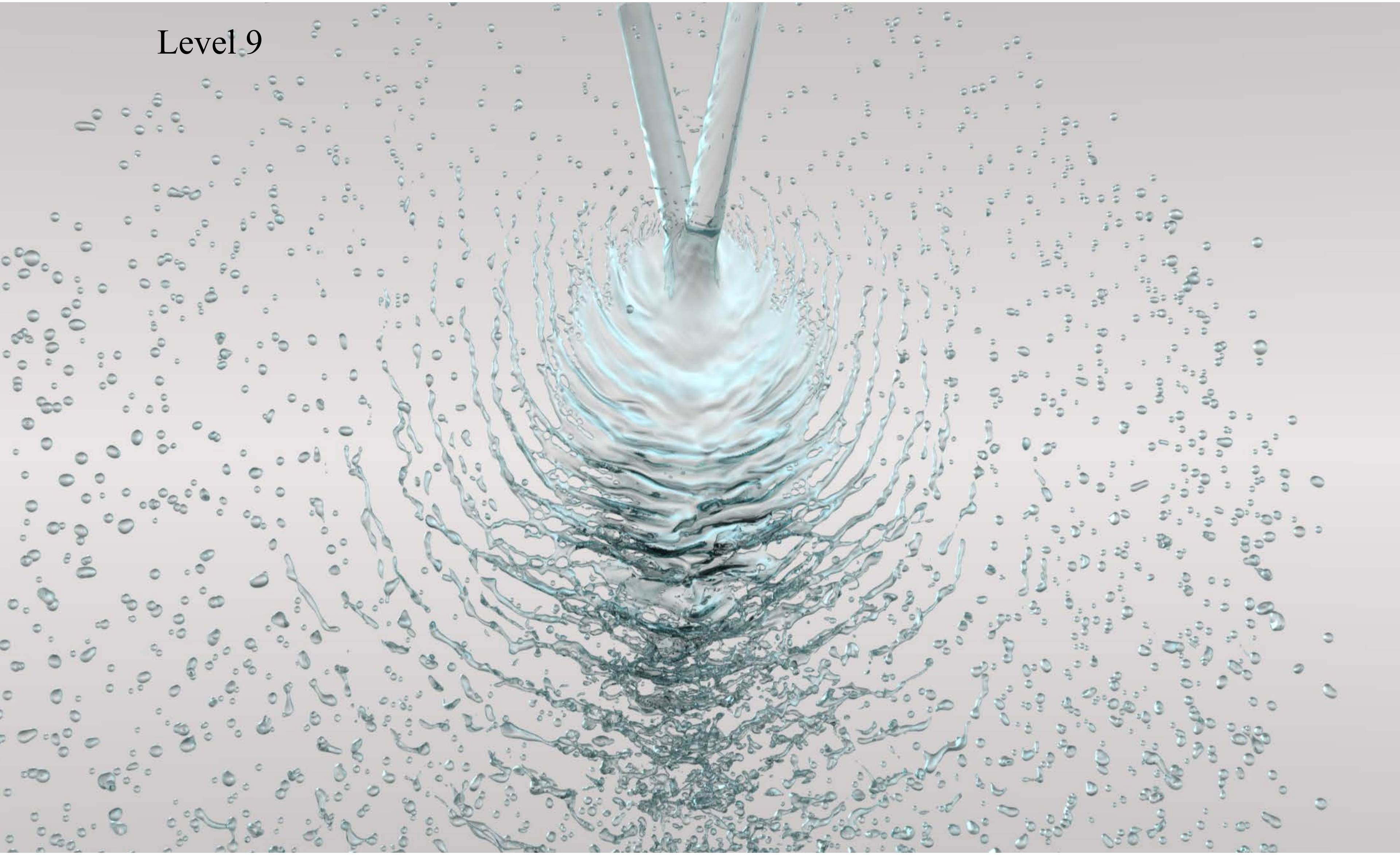

Atomization Under Different Grid Resolution

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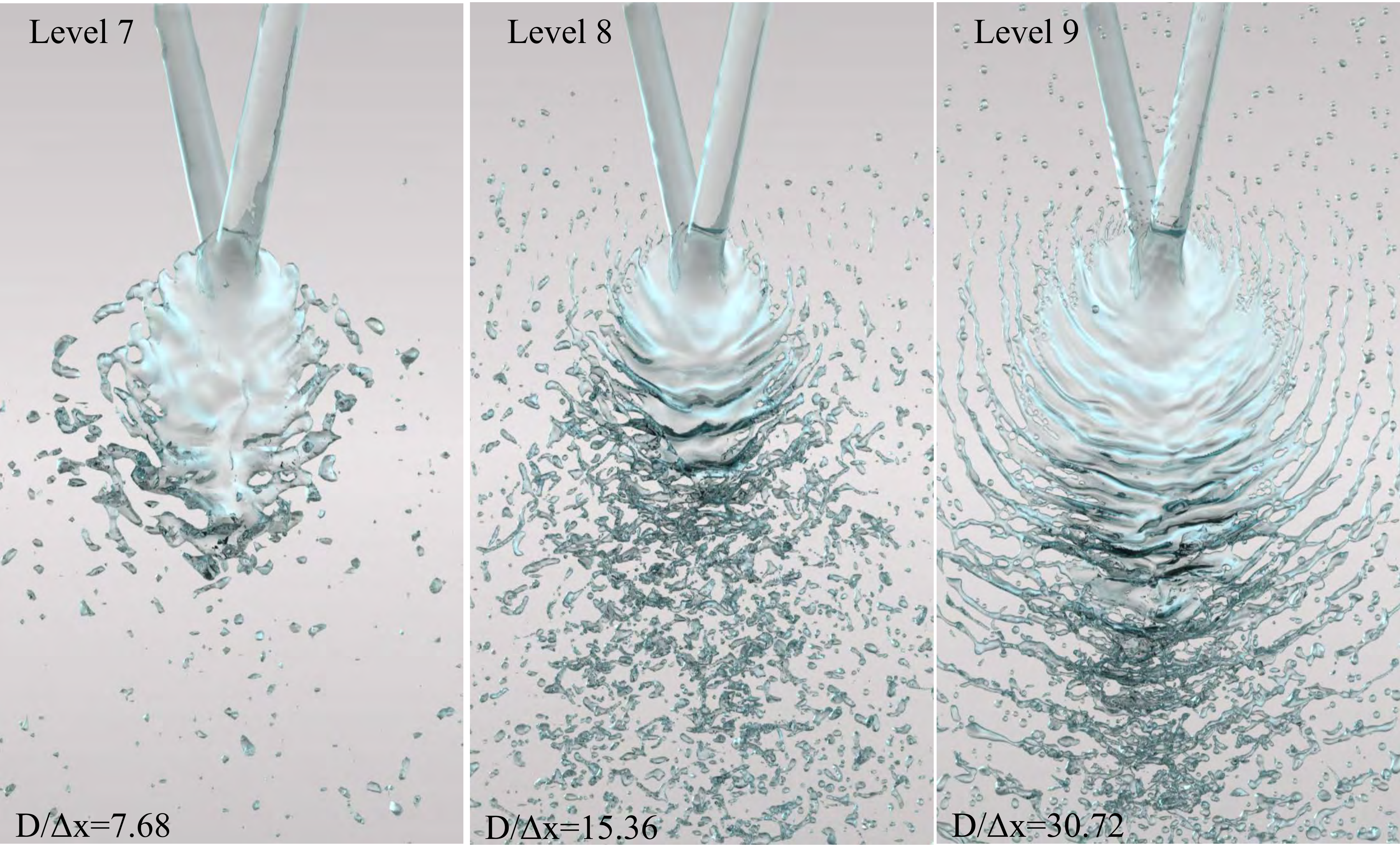
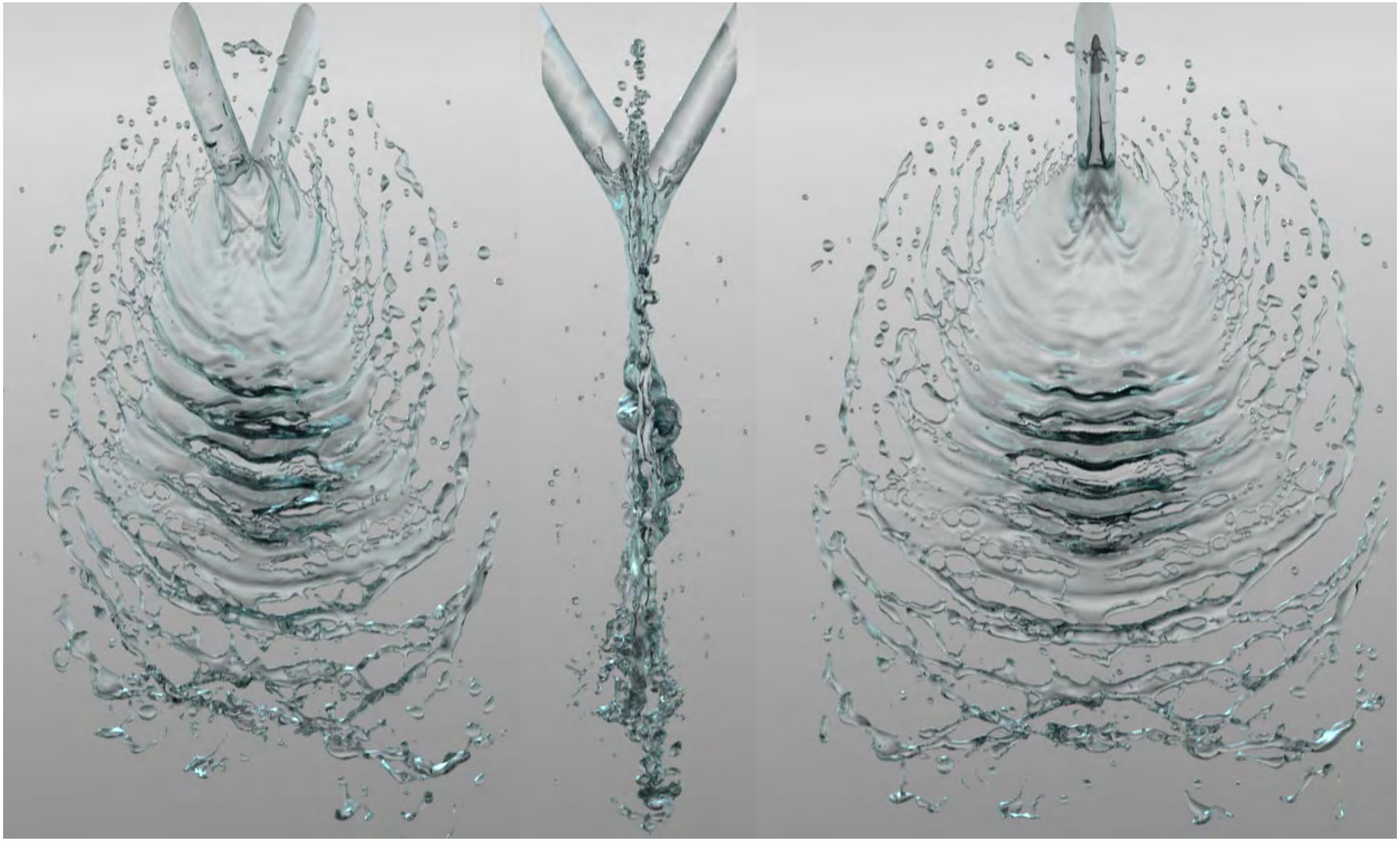
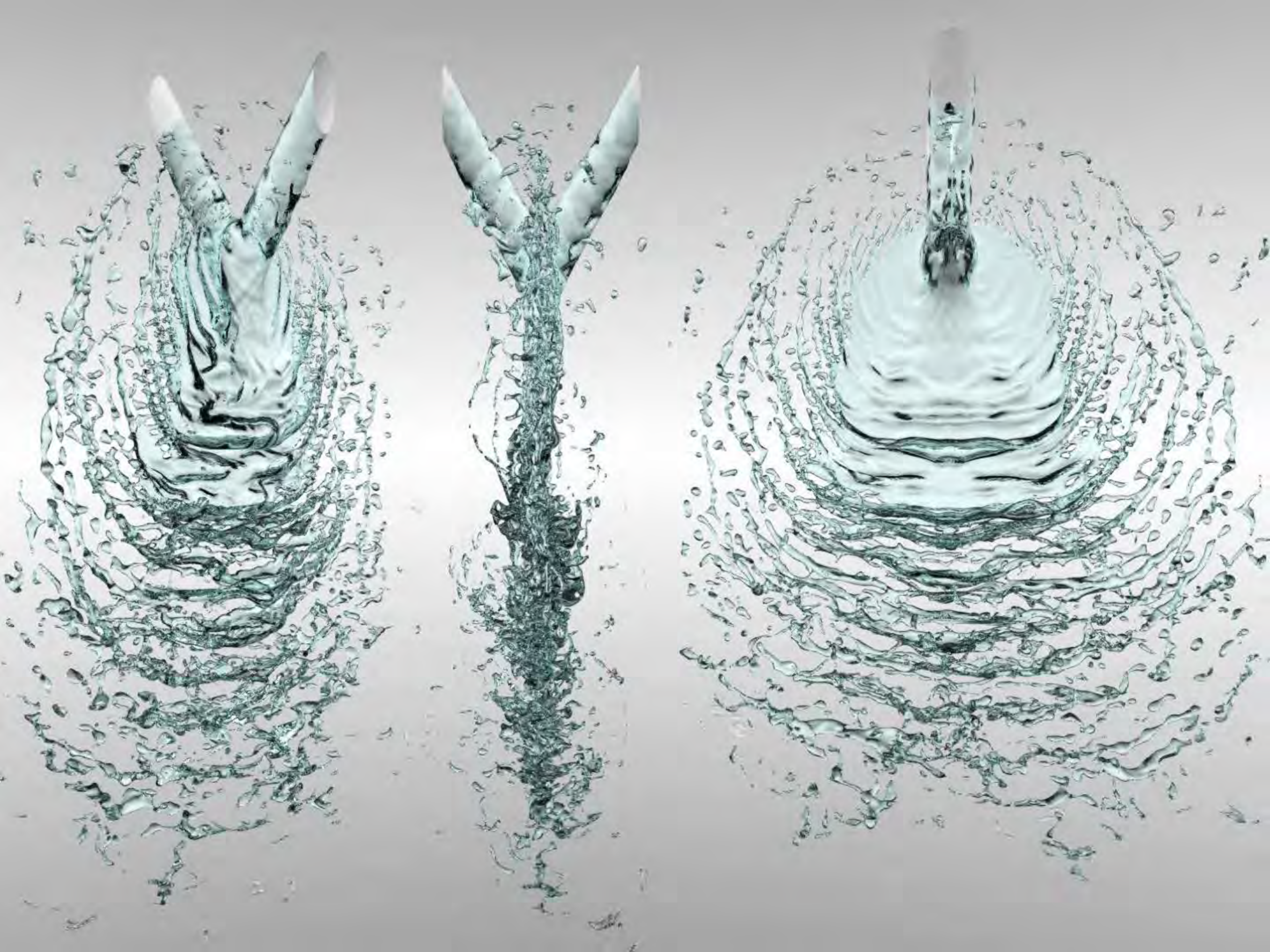


Impinging Jet Dynamics (GT Simulation)



Water Jets, D_j = 0.33 mm, V_j = 28 m/s, 2θ = 60º, Re = 9240, We = 3556



Probability Density Function of Droplet Size

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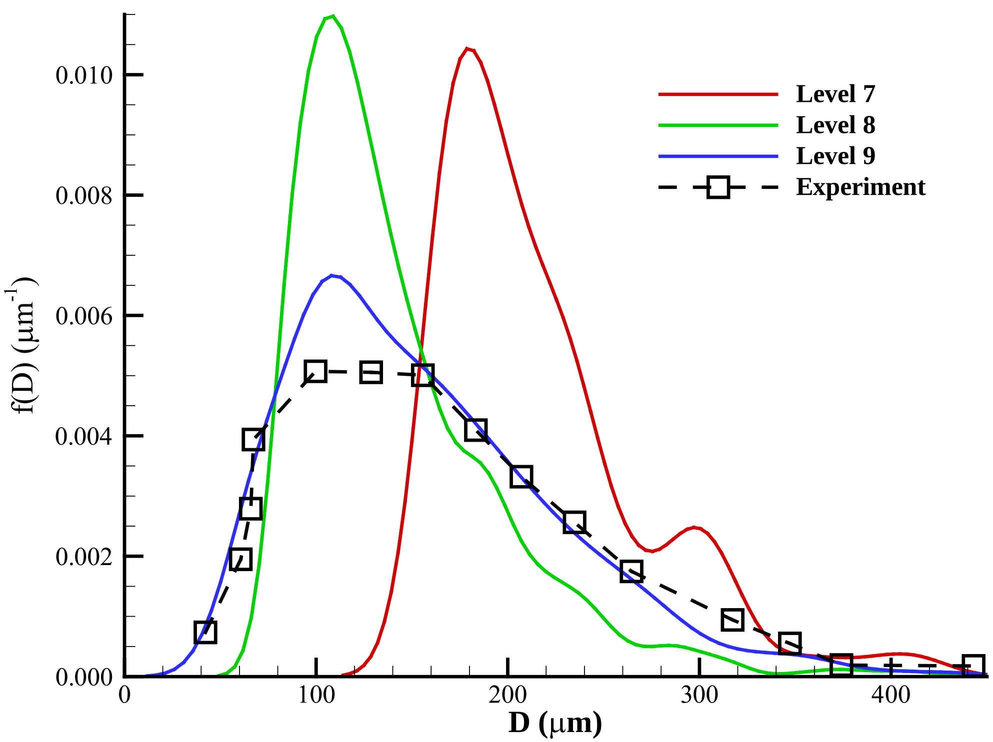
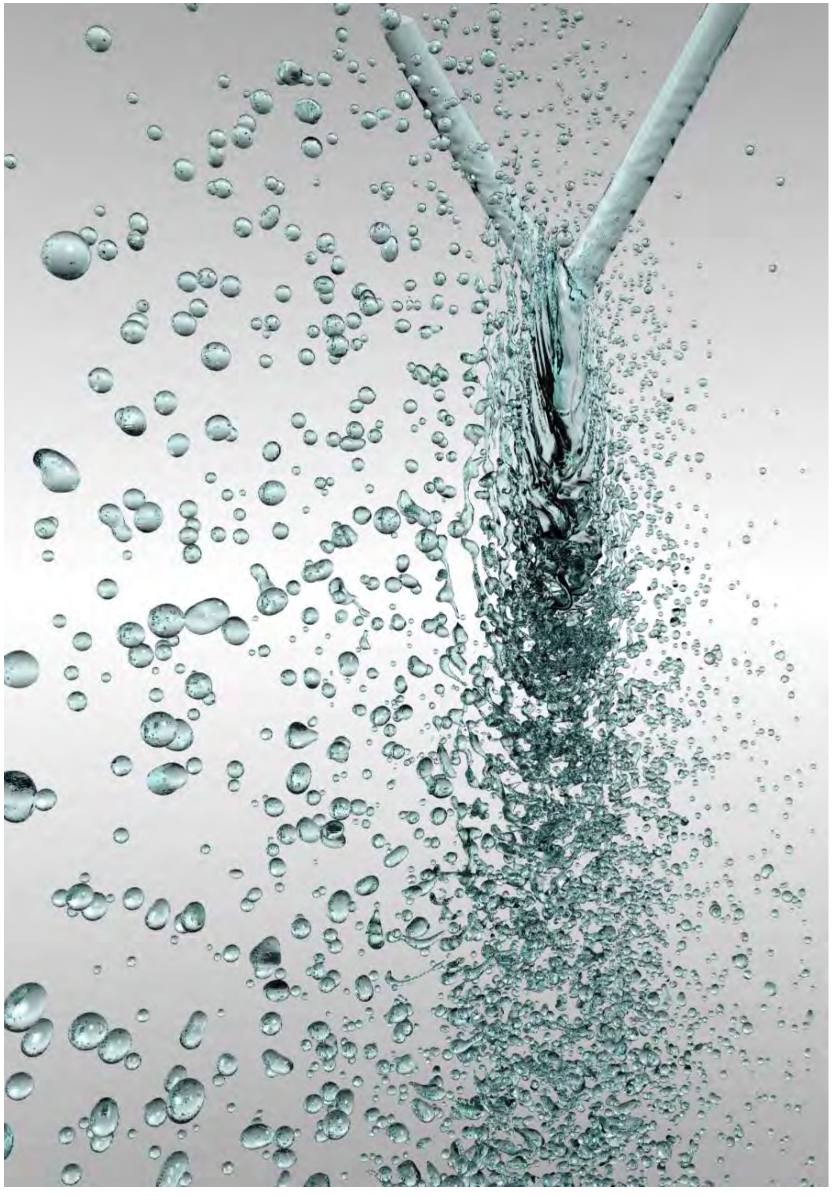
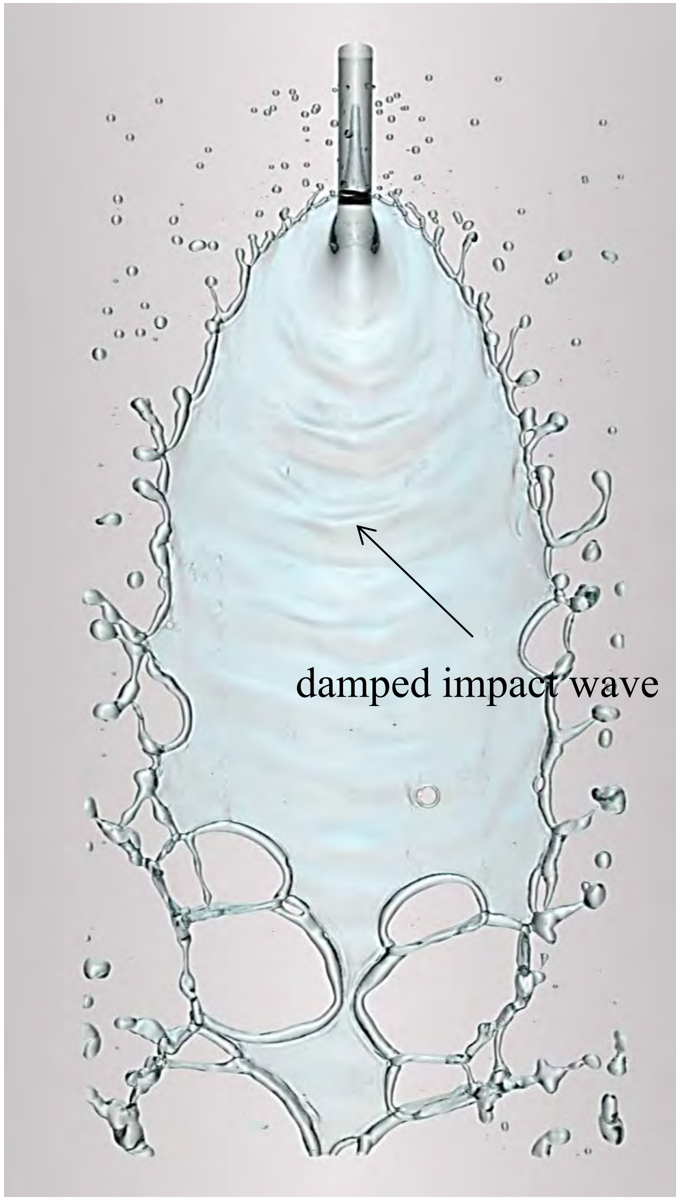




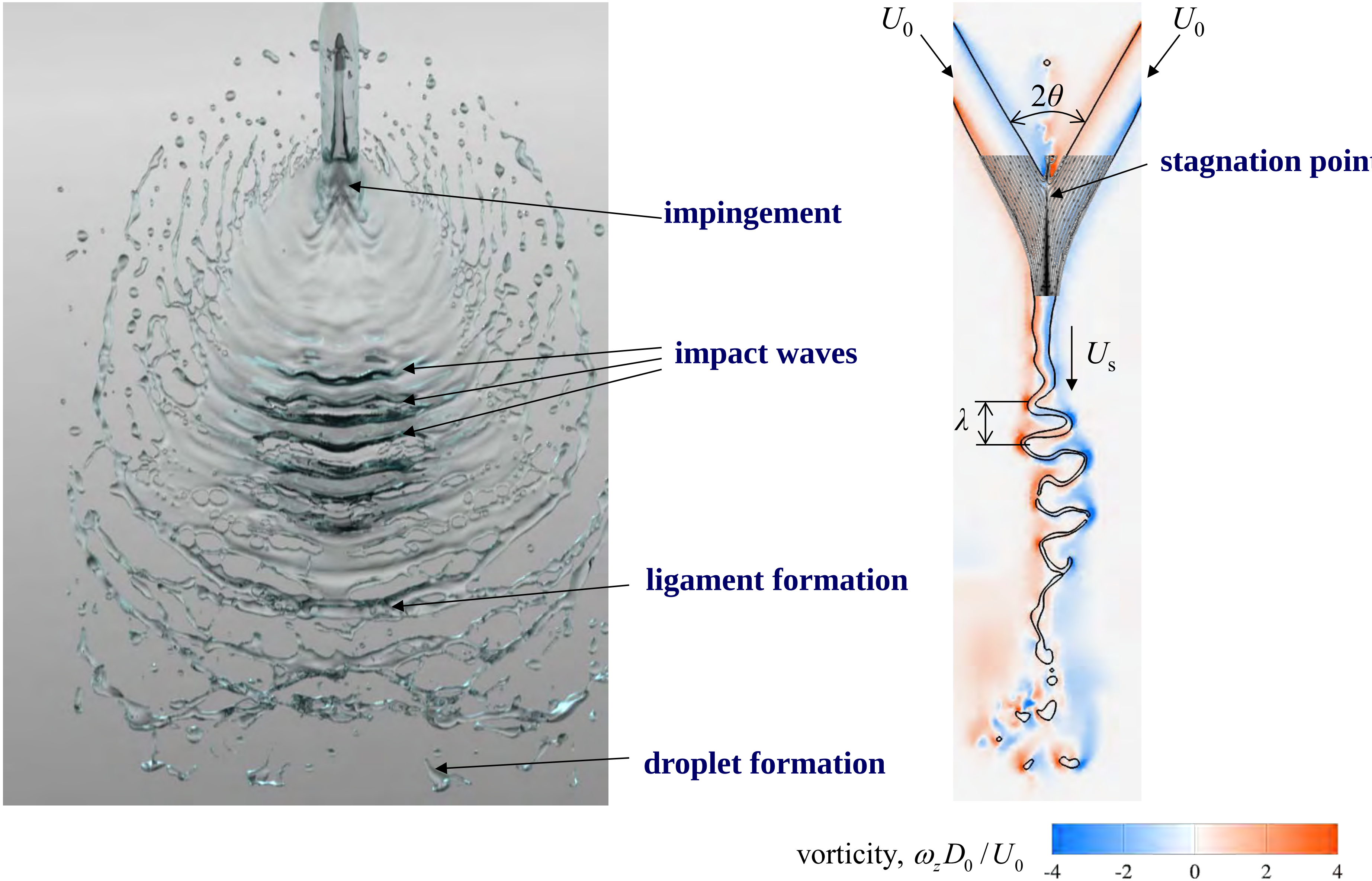
Ref: Atomization characteristics of impinging liquid jets, JPP 1995

Impact Wave



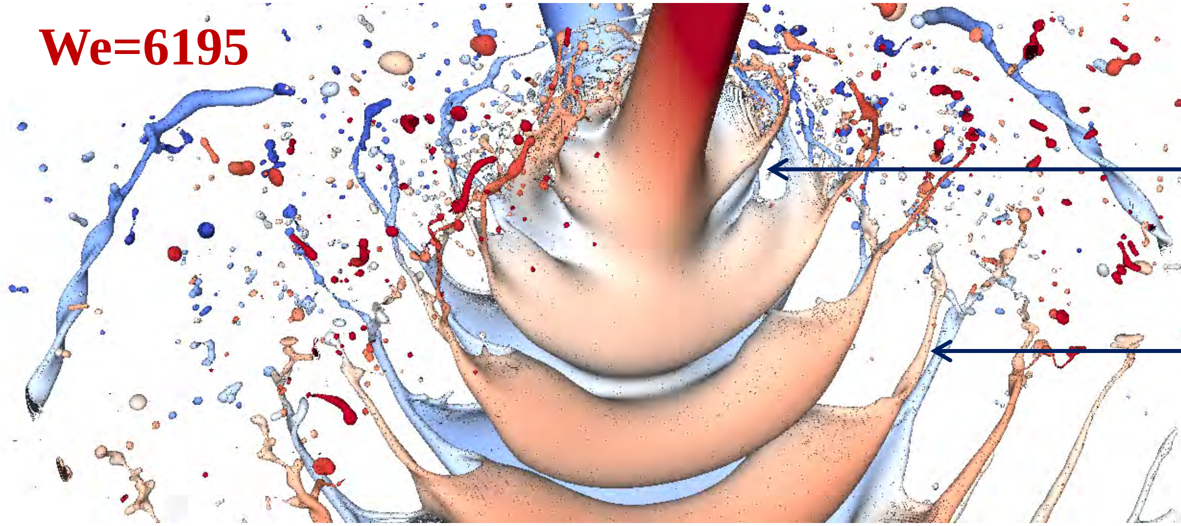
Breakup Caused by Impact Wave

Impinging Jet Dynamics



Impact-wave-induced Atomization

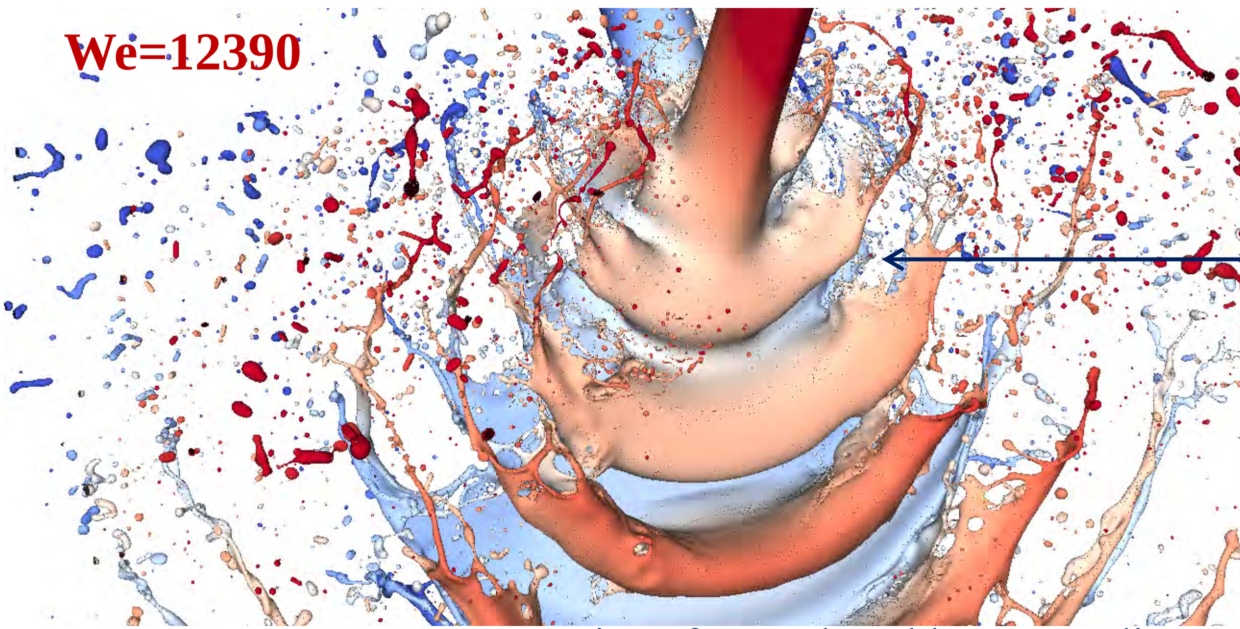
We=6195



breakup happens between wave crest and trough

ligaments locate along wave crest and trough

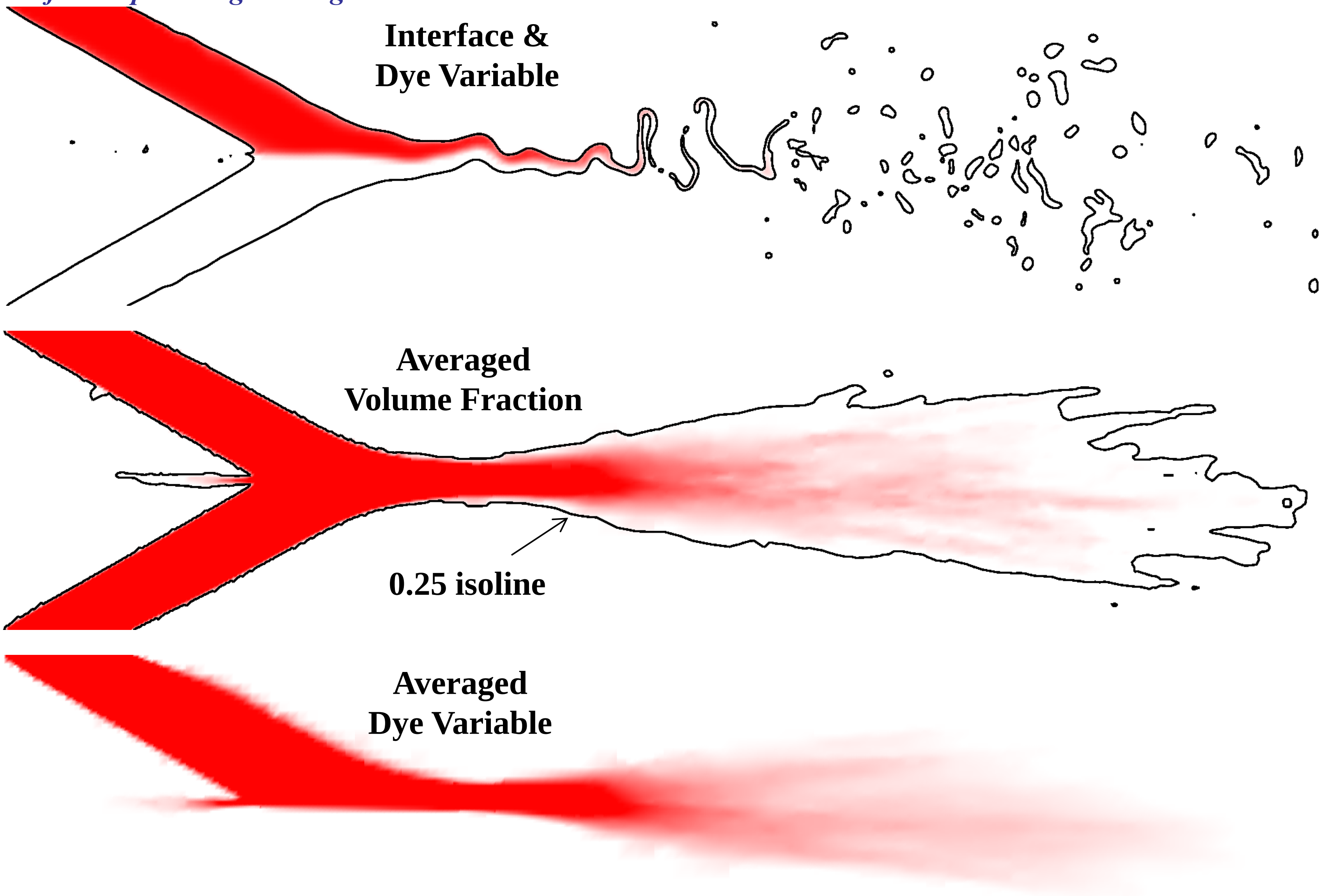
We=12390



complex breakup of liquid sheet

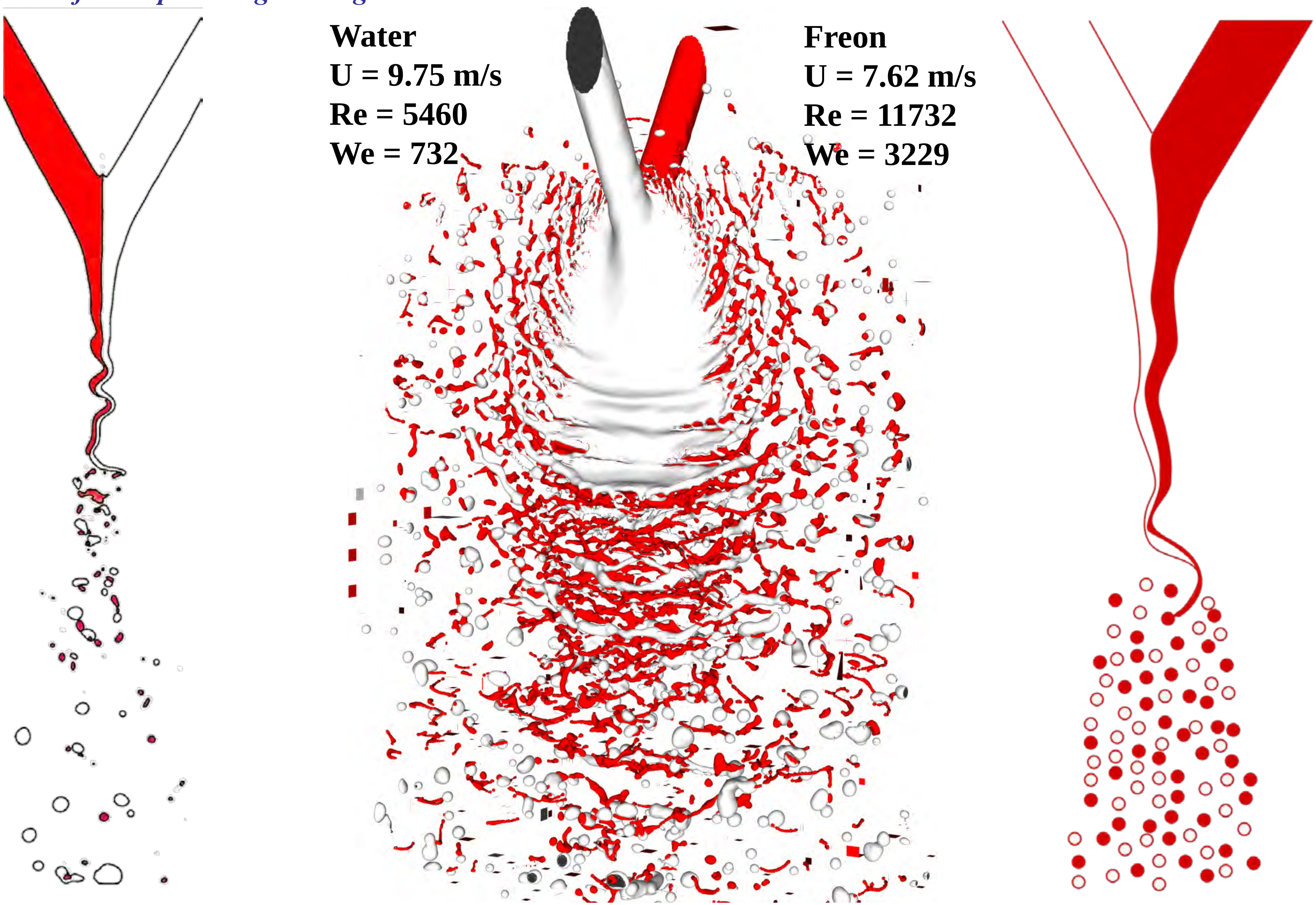
interface colored by z coordinate

Impact Wave Enhanced Mixing



Ref: Mixing mechanisms in a pair of impinging jets, JPP 2001

Impact Wave Enhanced Mixing

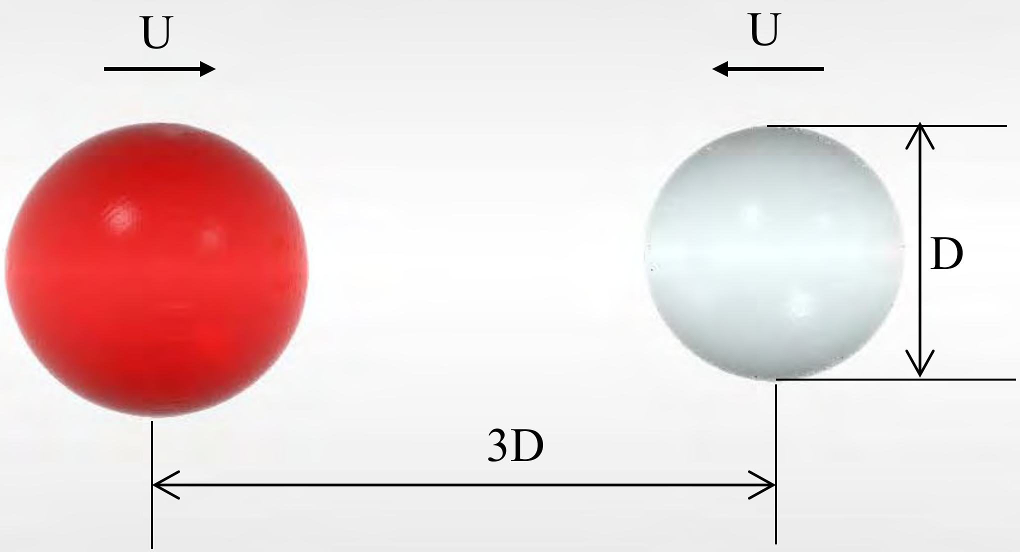


Ref: High Performance N2O4/AMINE Elements: Blowapart, *NASA CR-160273*, 1979

Tetradecane Droplets in 1 atm. Nitrogen

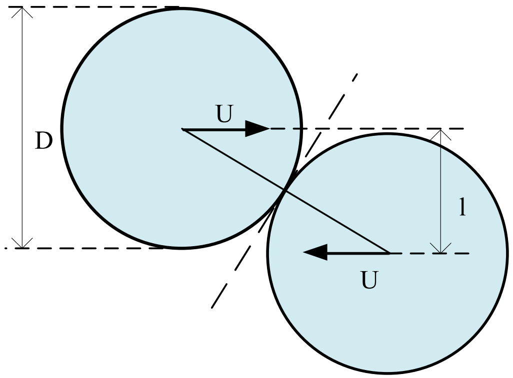
Density Ratio: 666 Viscosity Ratio: 119

Domain: 3D×3D×9D



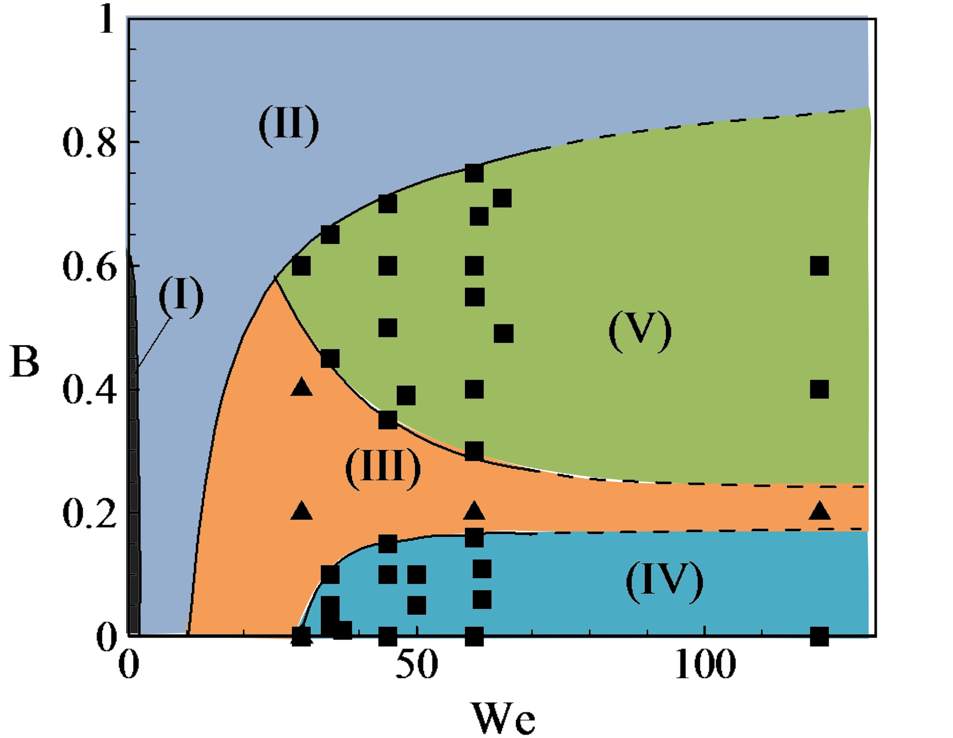
24 CPUs
about 600,000 AMR grids with load-balancing
equivalent to about 50,000,000 fixed sized grids

Regimes of Coalescence and Separation



Weber Number $We = \dfrac{\rho D (2U)^2}{\sigma}$

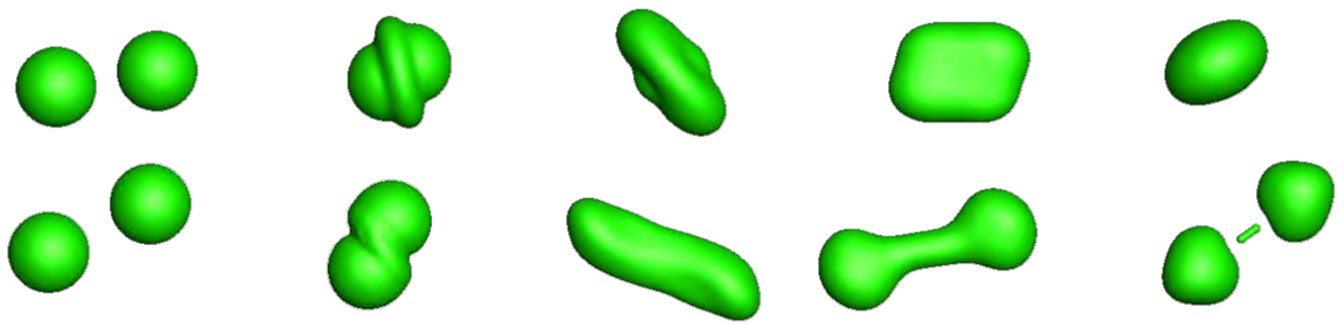
Impact Parameter $B = l / D$



(I) coalescence after minor deformation, (II) bouncing, (III) coalescence after substantial deformation, (IV) reflexive separation, (V) stretching separation

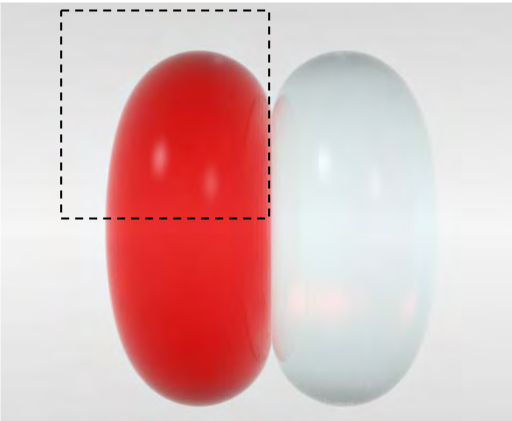
Coalescence ▲

Separation ■

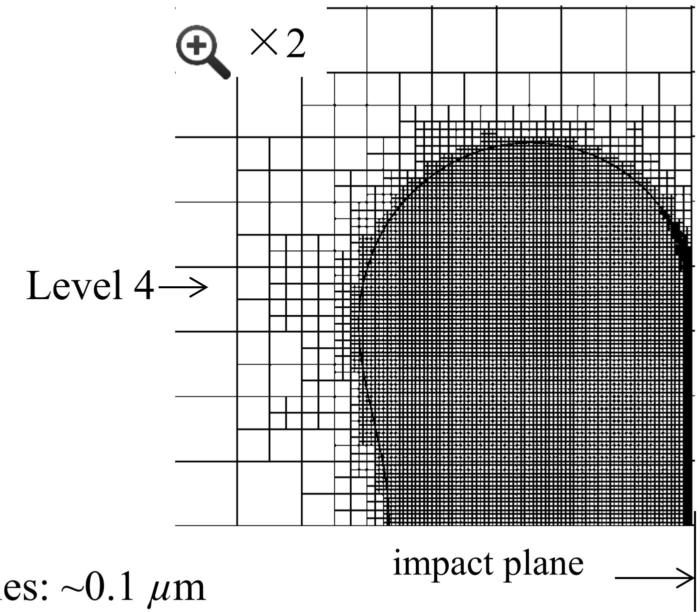


Ref: Qian, J. and Law, C.K. Regimes of coalescence and separation in droplet collision. *Journal of Fluid Mechanics*, 1997, **331**(-1), 59-80.

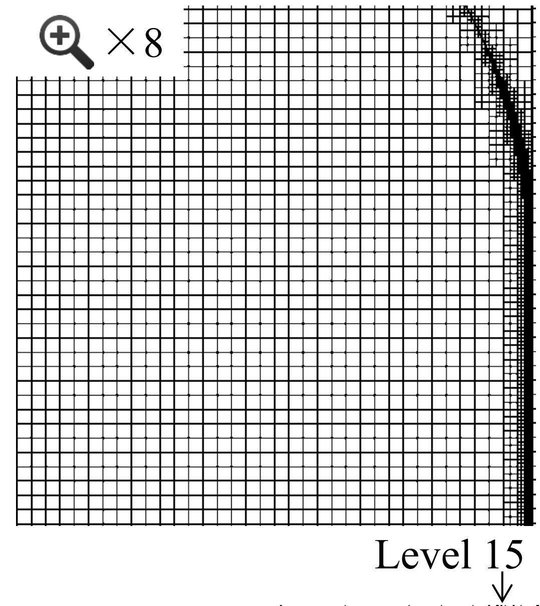
Grid Resolution at Max Deformation

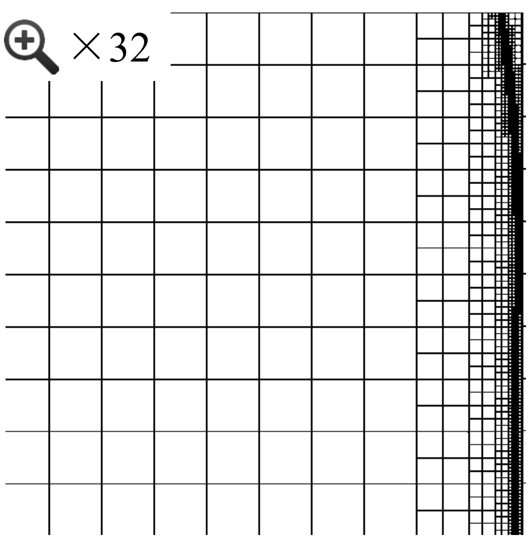


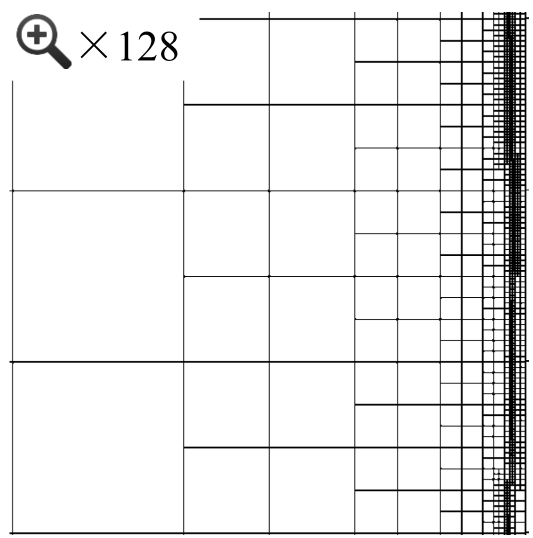
droplet diameter : 300 μm
max resolution : 0.015 μm
mean free path of gas molecules: ~0.1 μm
Van der Waals force affect distance: ~0.03 μm

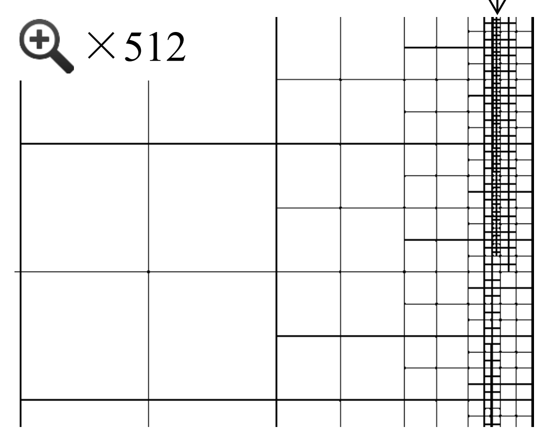


thickness-based refinement



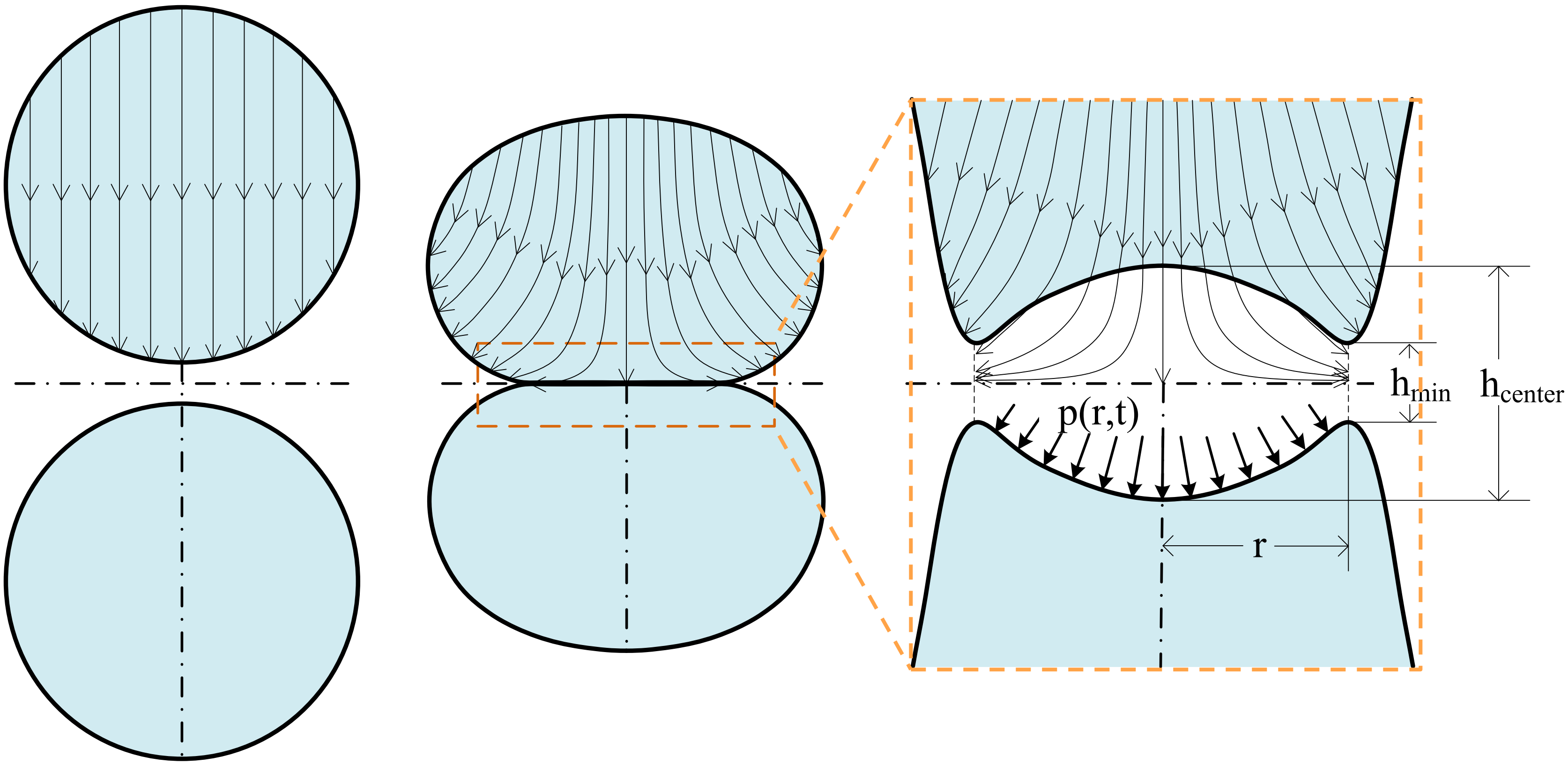






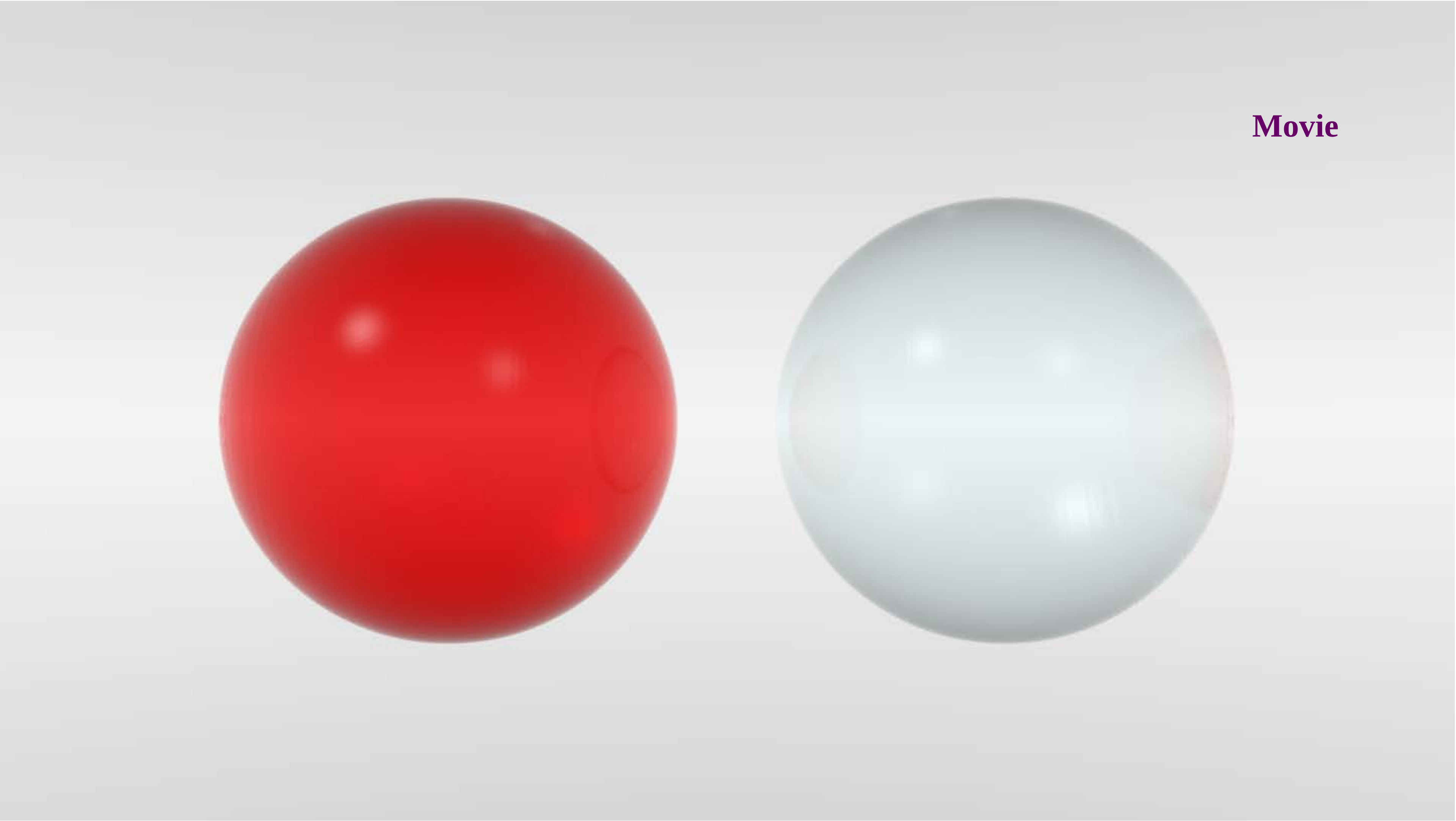
at least 3~5 grids in gas film to
catch lubrication dynamics

Effect of Gas Film Lubrication

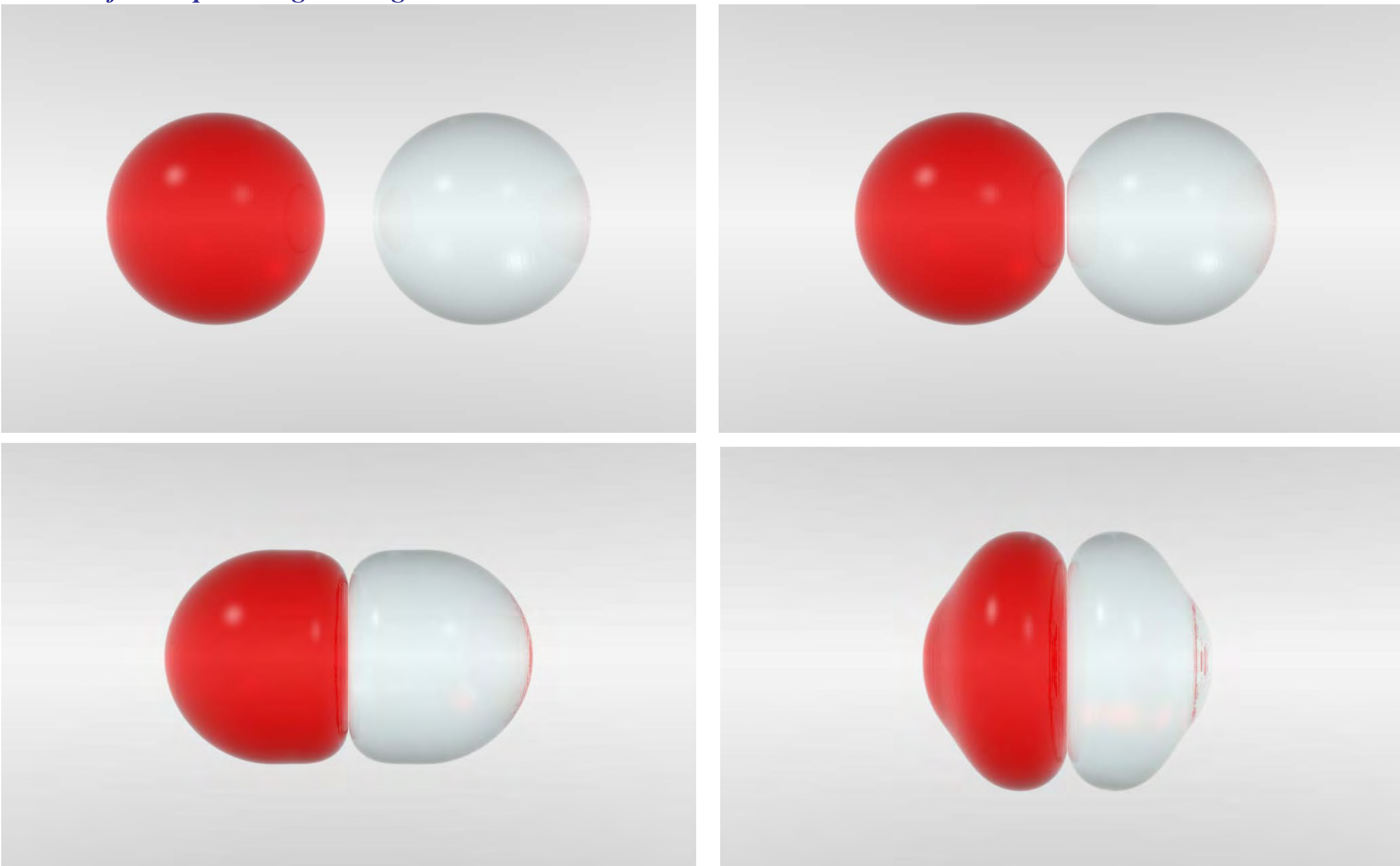


- The pressure generated within the film will prevent the motion of the approaching droplets.
- The normal component of collision motion is normal squeeze action that provides a valuable cushioning effect when the surfaces of the two droplets tend to be pressed together.
- It is known from "Reynolds equation" which governing the pressure distribution in fluid film lubrication that the pressure is maximum at the center and minimum at the boundary.

Head-on Bouncing

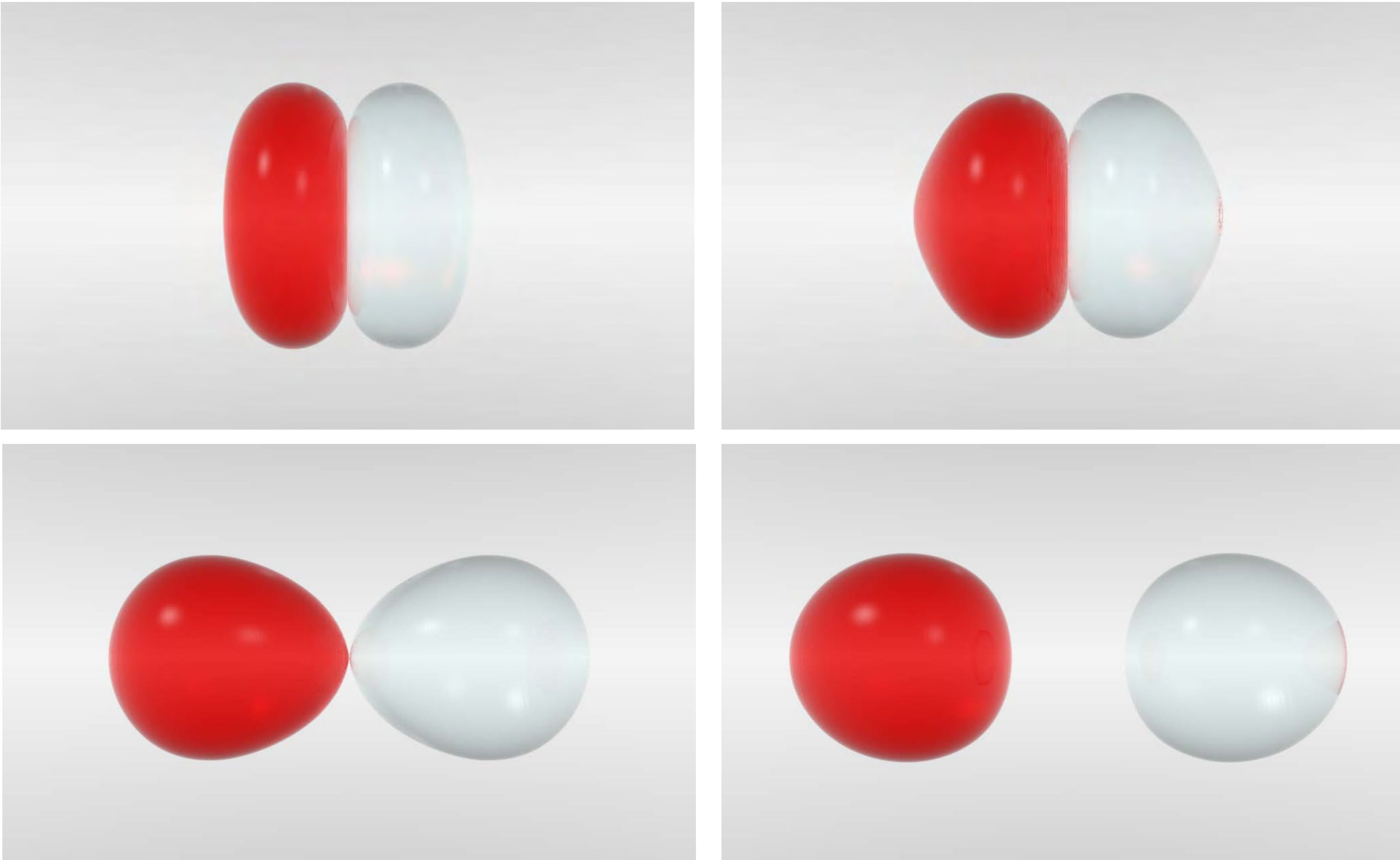


Droplet Bouncing



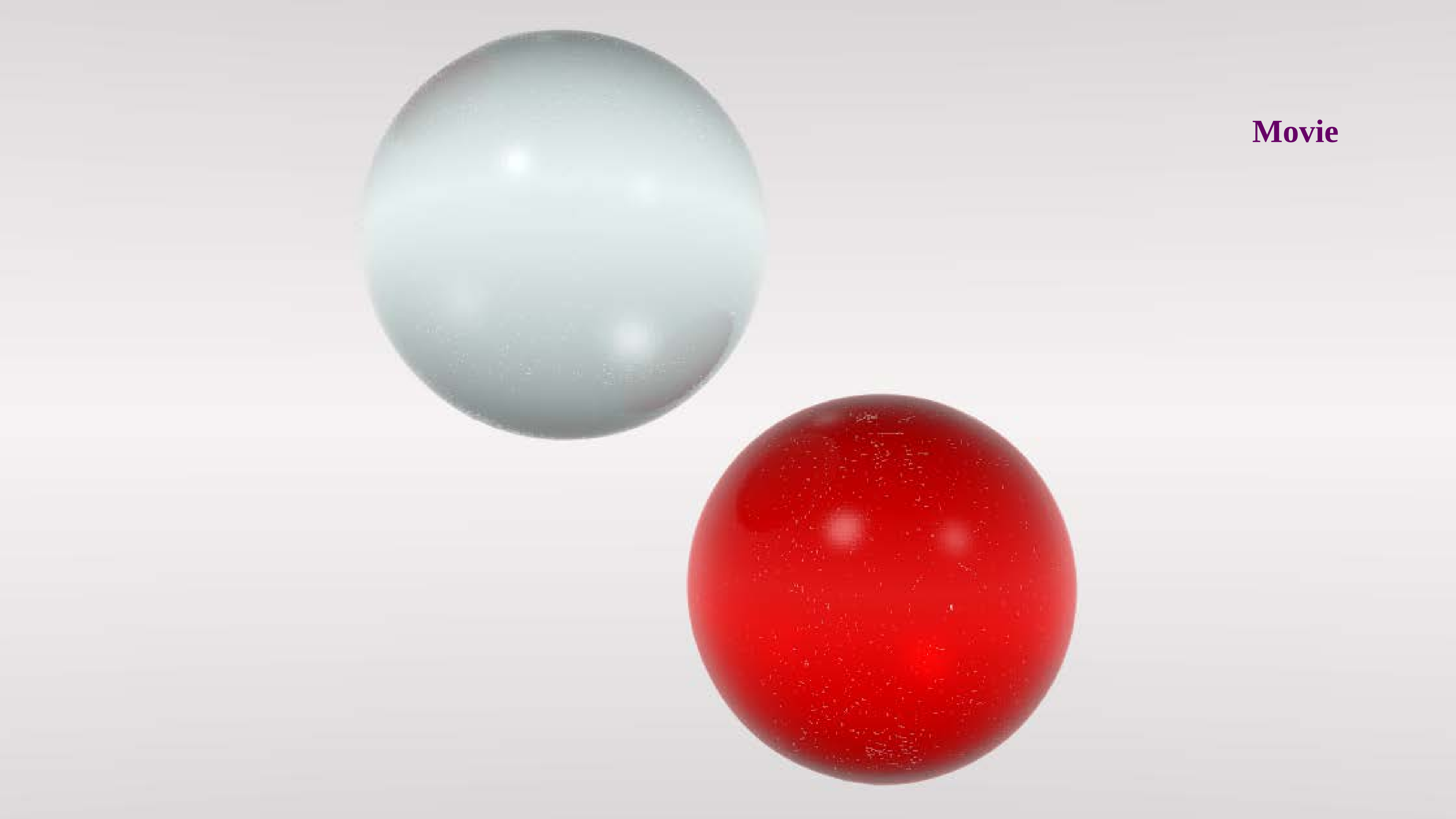
We=8.6, Re=105.9, B=0.0, D=306 μm, U=0.97 m/s, ρ=758 kg/m^3, μ= 2.13$\times$10^{-3} N·s/m^2

Droplet Bouncing



We=8.6, Re=105.9, B=0.0, D=306 μm, U=0.97 m/s, ρ=758 kg/m^3, μ= 2.13×10^{-3} N·s/m^2

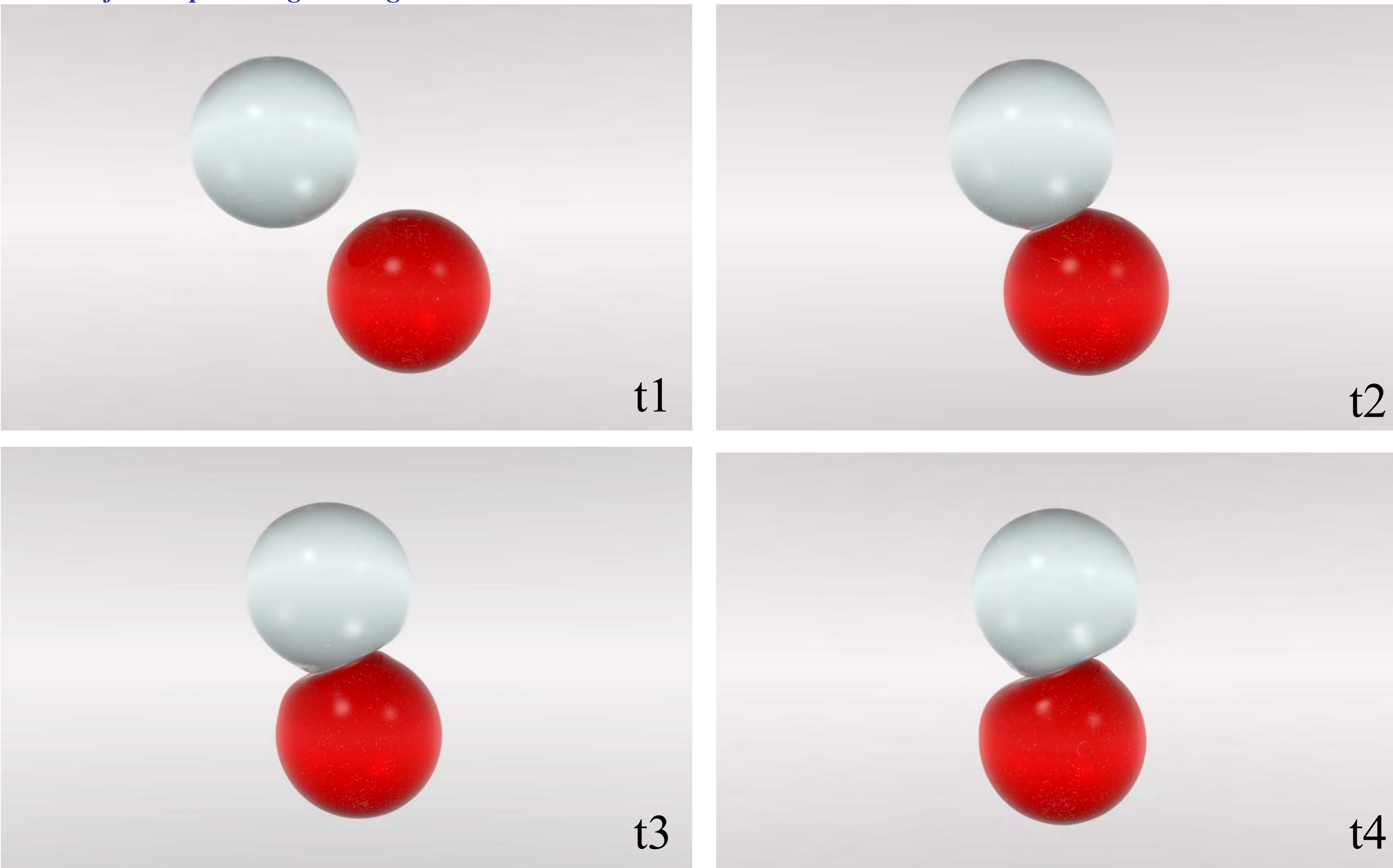
Off-center Droplet Bouncing



Movie

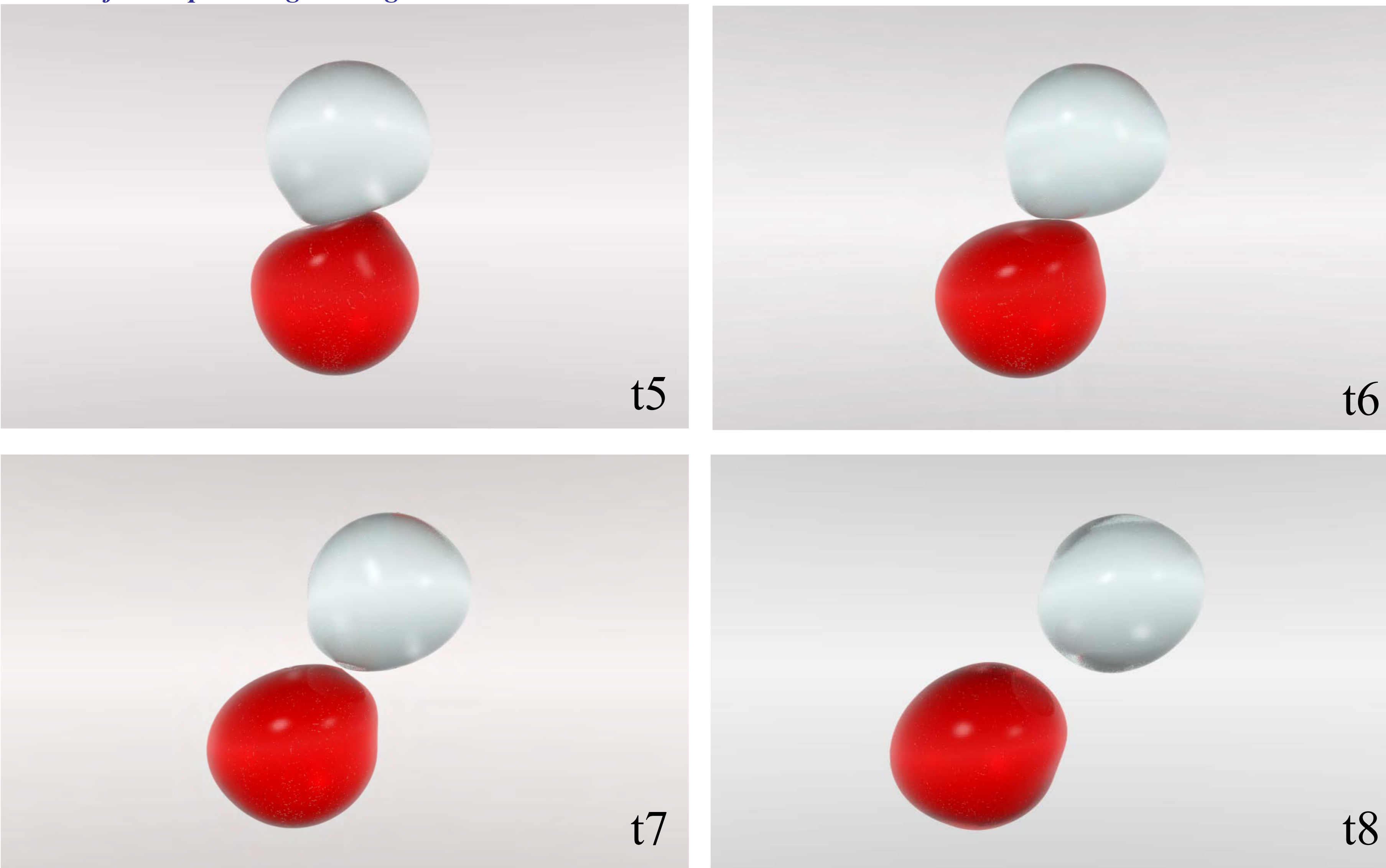
We=48.8, Re=260.3, B=0.9, D=306 μm, U=2.31 m/s, ρ=758 kg/m^3, μ= 2.13$\times$10^{-3} N·s/m^2

Off-center Droplet Bouncing



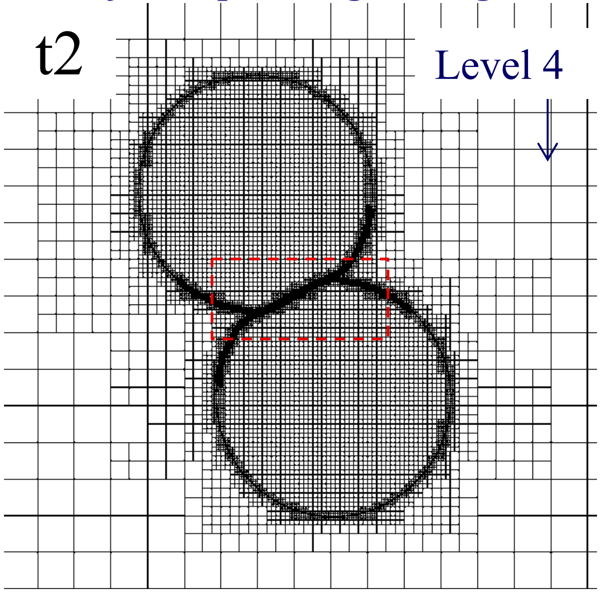
We=48.8, Re=260.3, B=0.9, D=306 μm, U=2.31 m/s, ρ=758 kg/m^3, μ= 2.13$\times 10^{-3}$ N·s/m^2

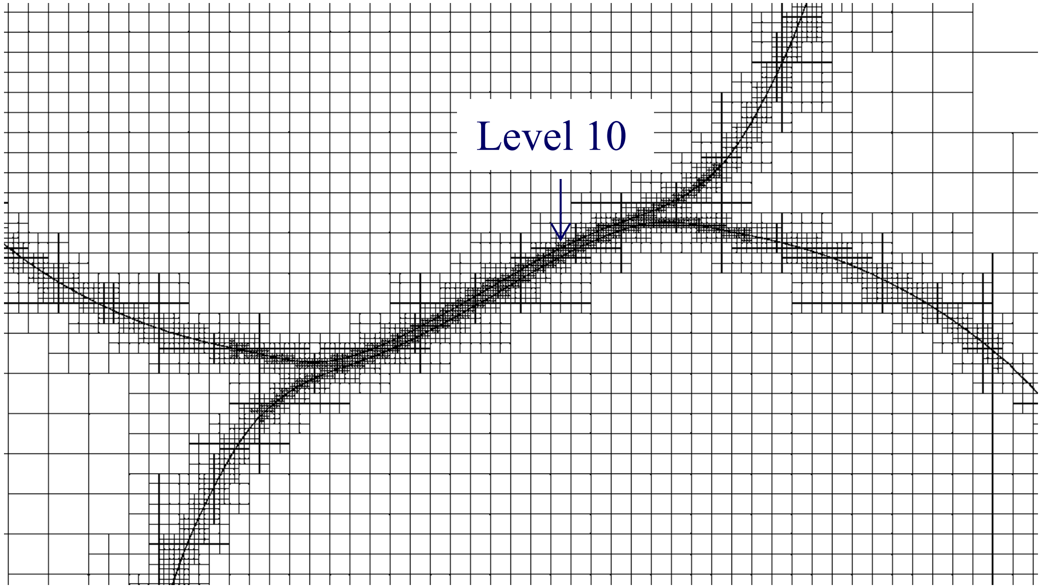
Off-center Droplet Bouncing

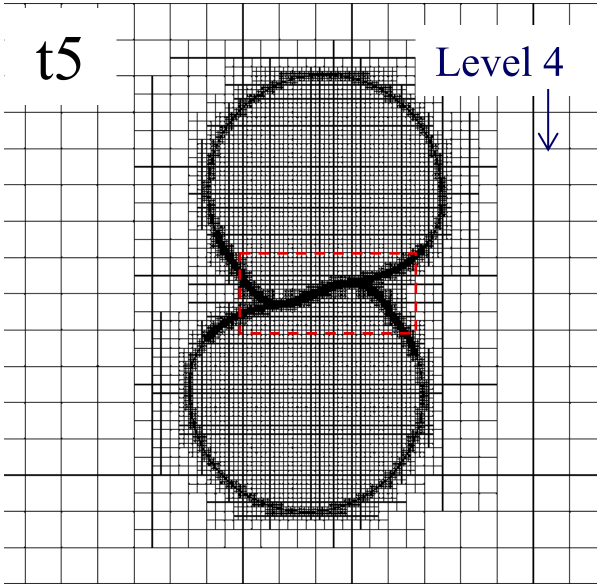


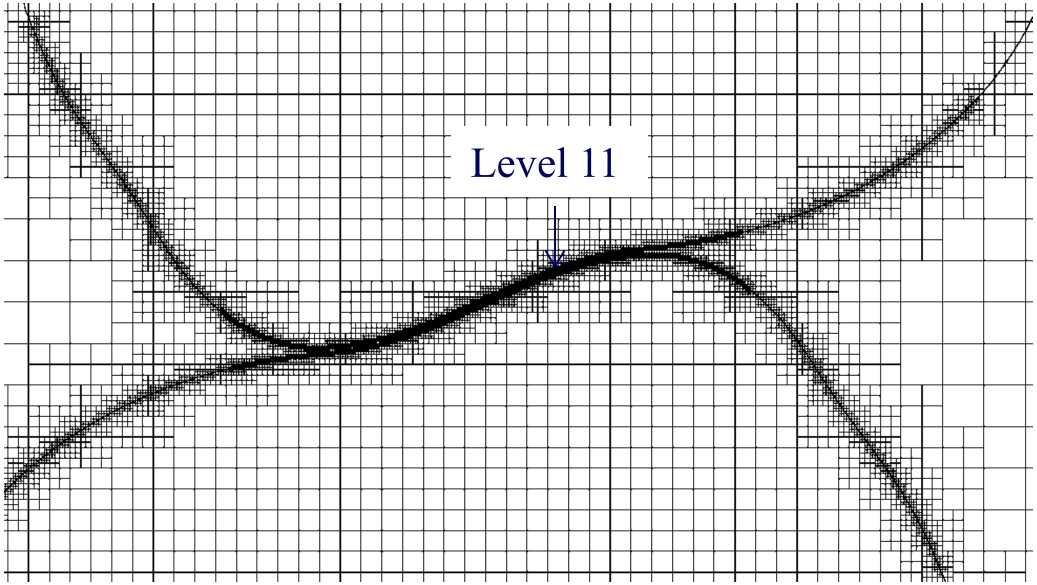
We=48.8, Re=260.3, B=0.9, D=306 μm, U=2.31 m/s, ρ=758 kg/m^3, μ= 2.13$\times$10^{-3} N·s/m^2

Off-center Droplet Bouncing

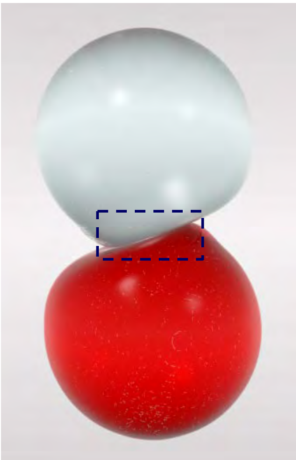


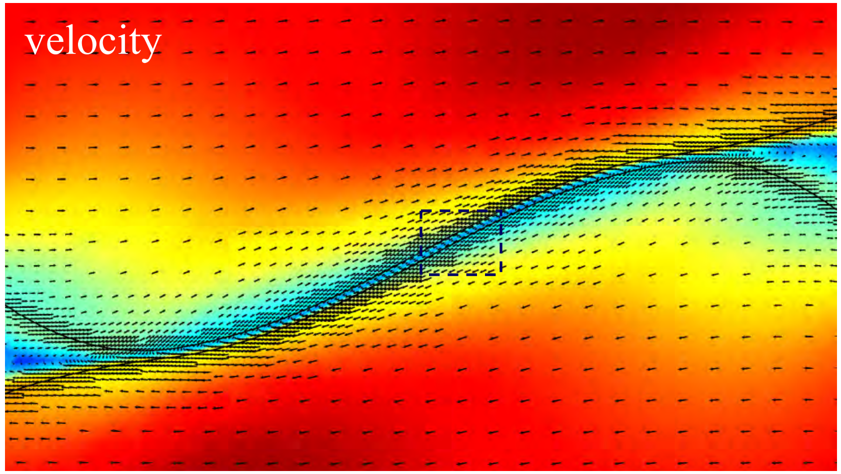


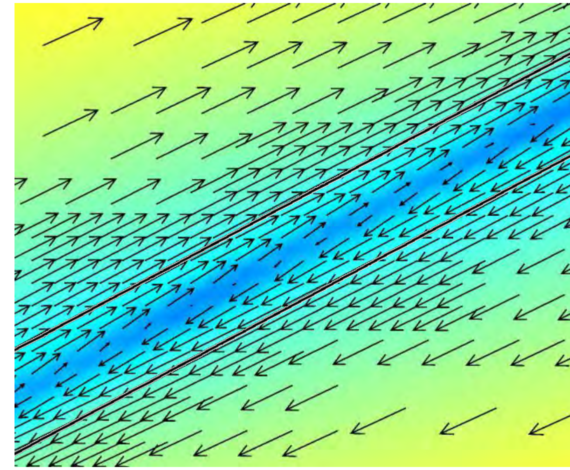


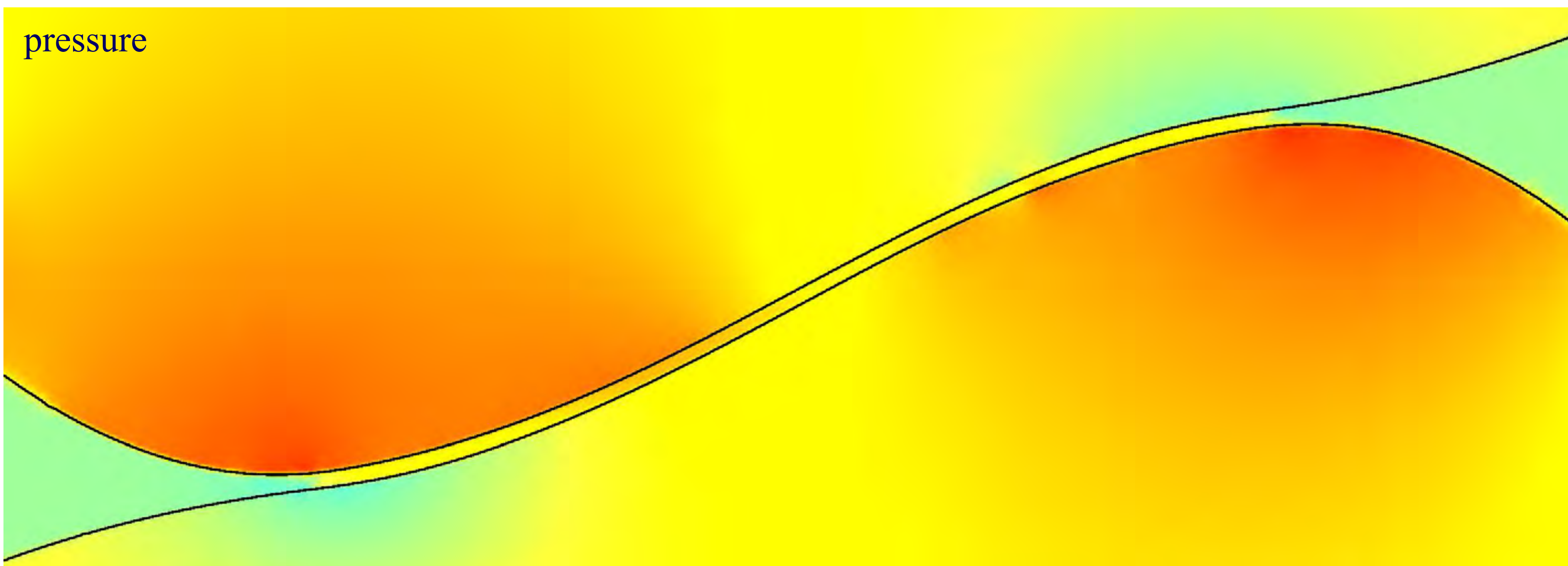


Pressure Buildup at Collision Plane









Georgia Tech

Droplet Collision & Reflexive Separation

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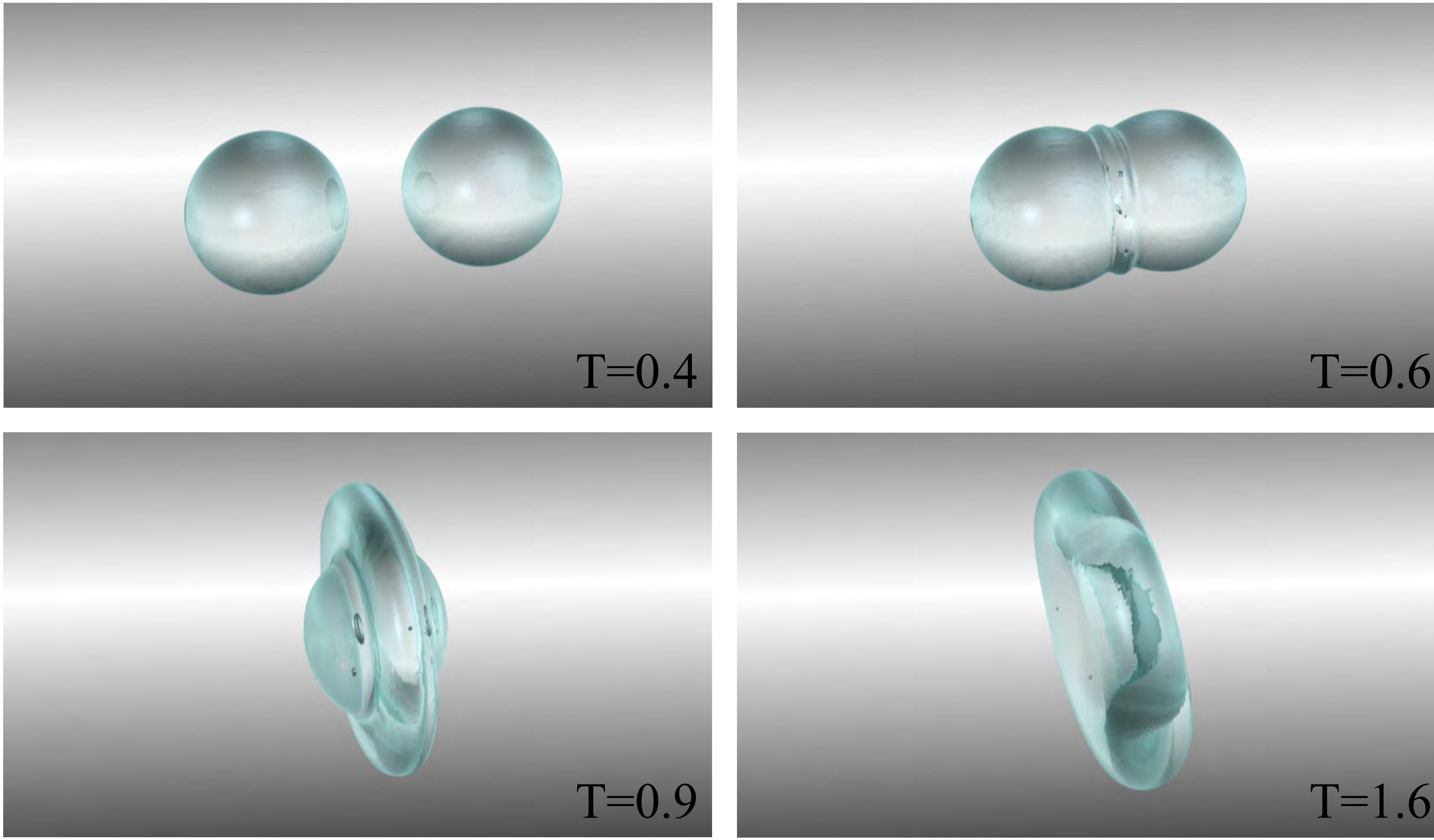
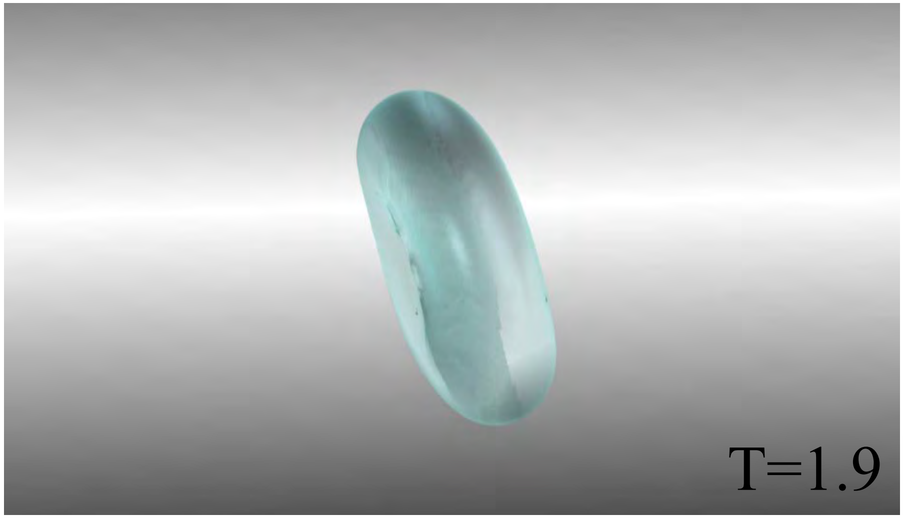
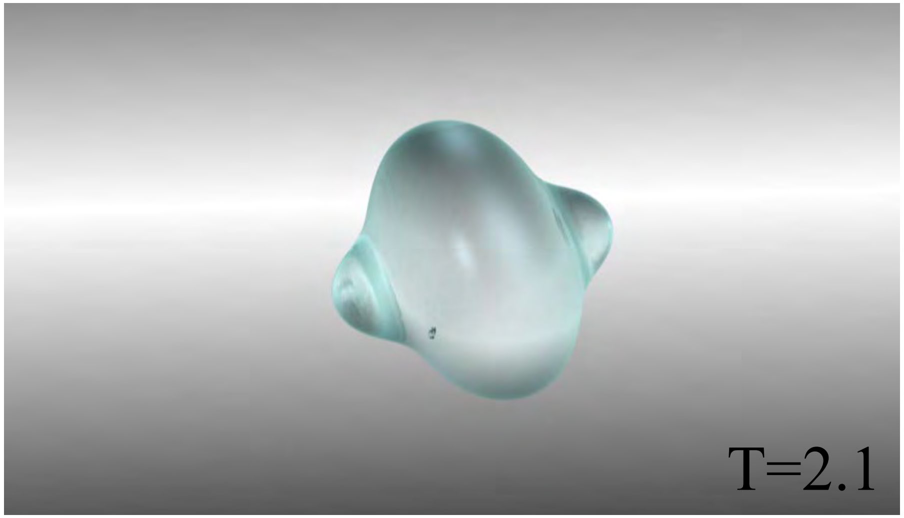
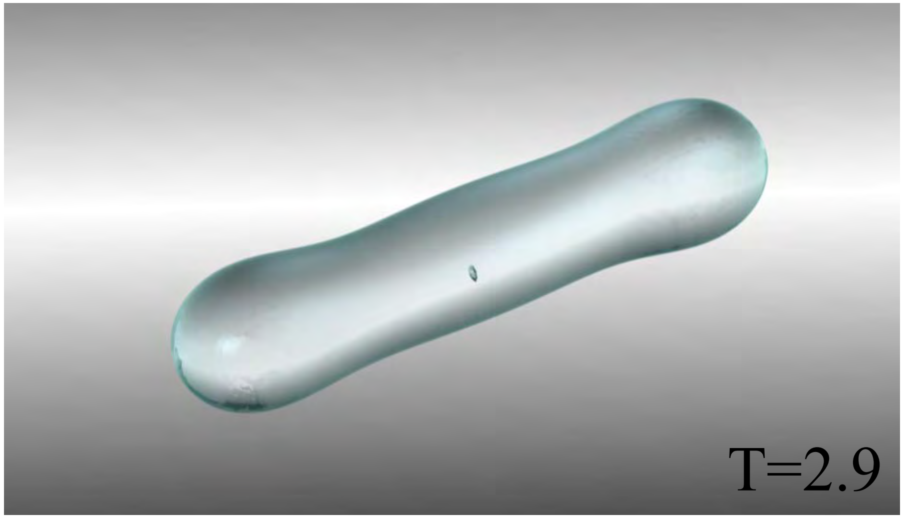


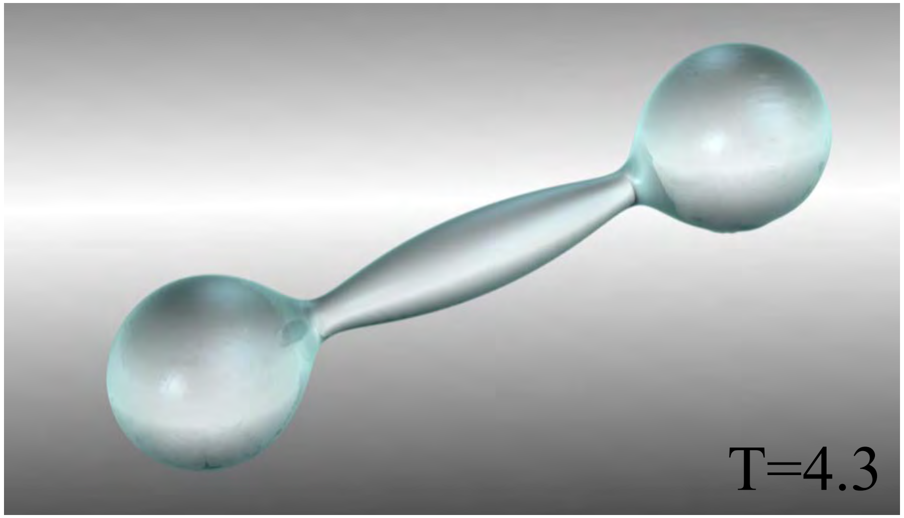
We=61.4, Re=296.5, B=0.06, D=336 μm, U=2.48 m/s, ρ=758 kg/m^3, μ= 2.13$\times 10^{-3}$ N·s/m^2

Droplet Collision & Reflexive Separation

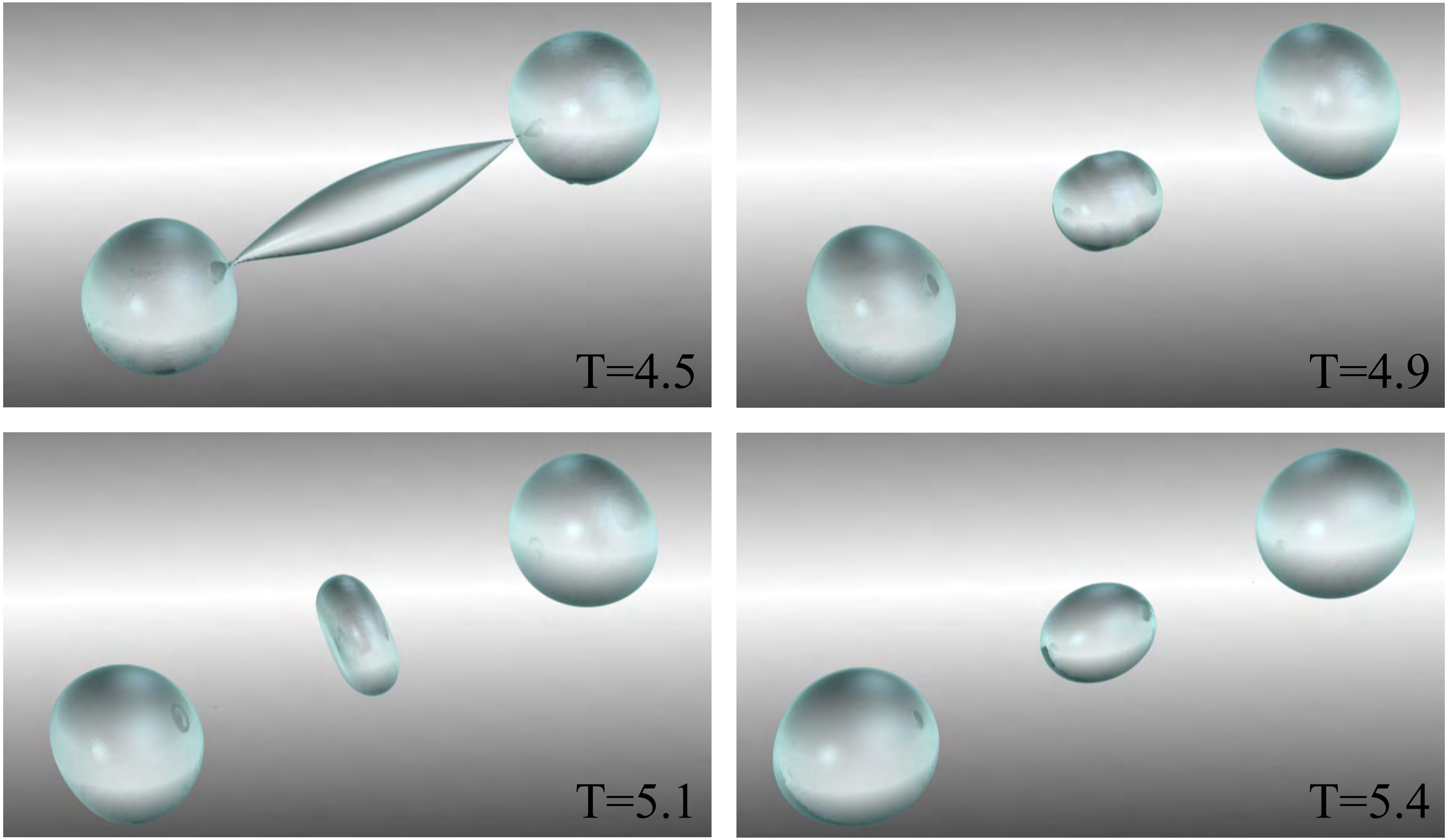






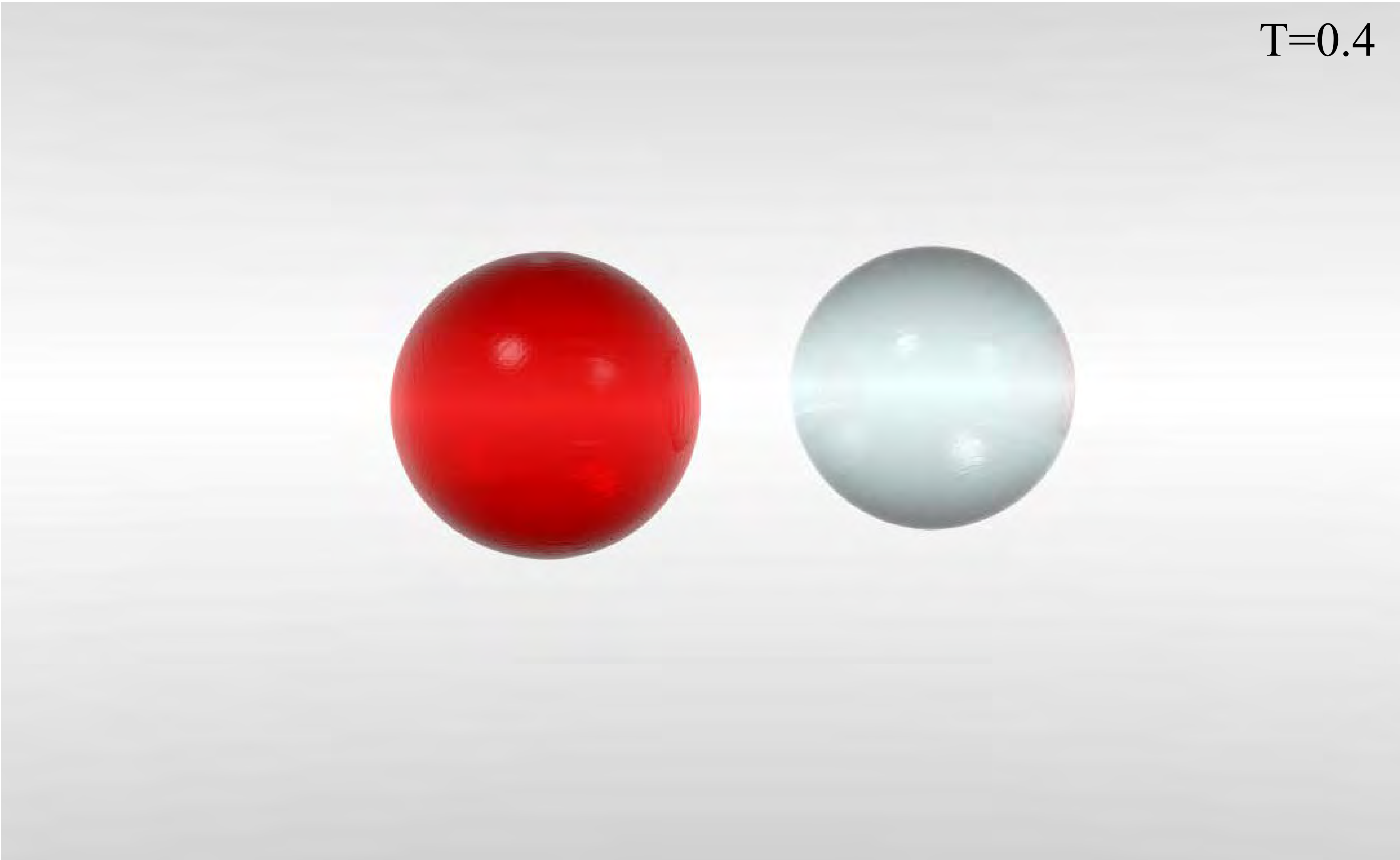


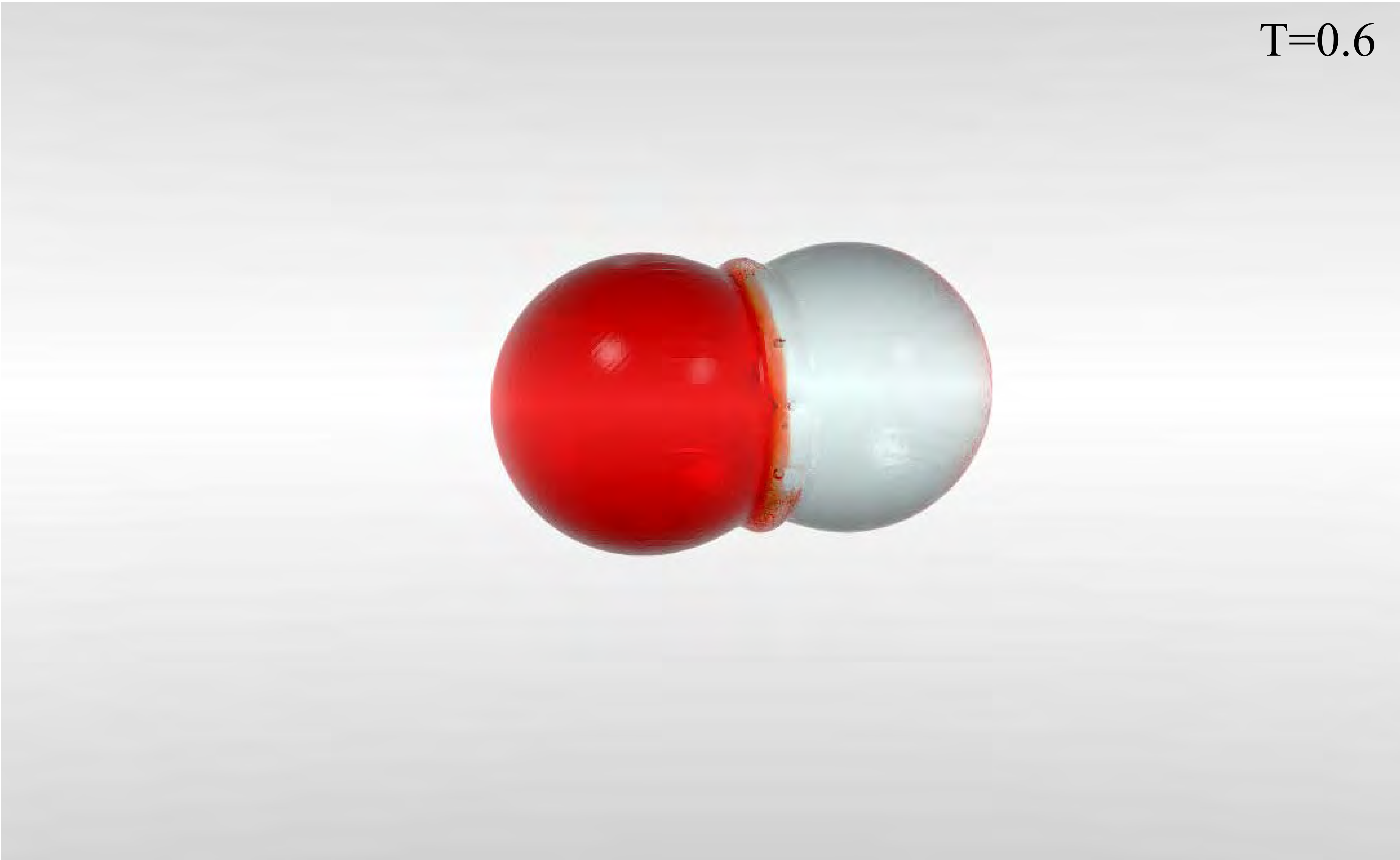
Droplet Collision & Reflexive Separation



Droplet Collision & Reflexive Separation

Movie


T=0.4

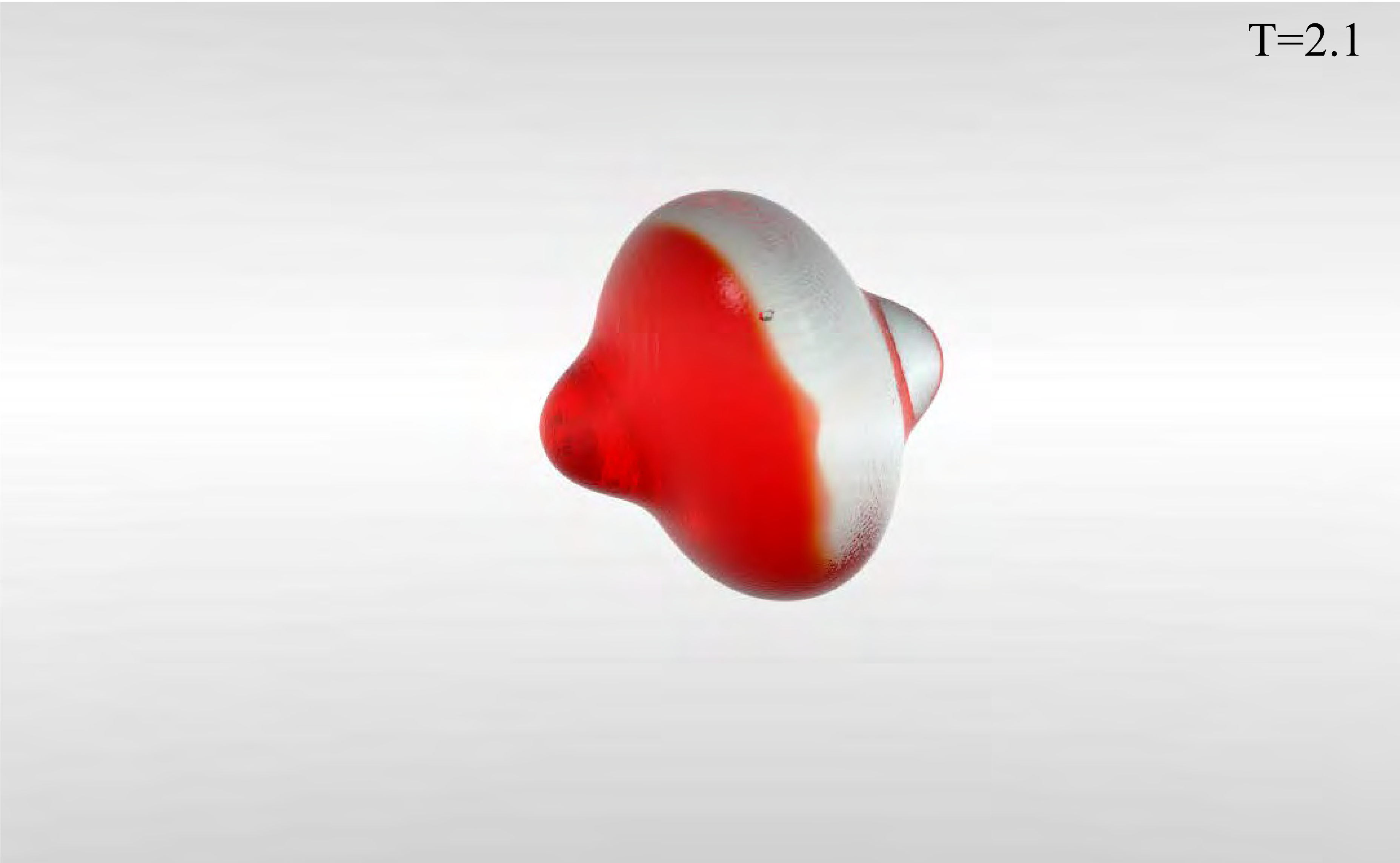

T=0.6


T=0.9

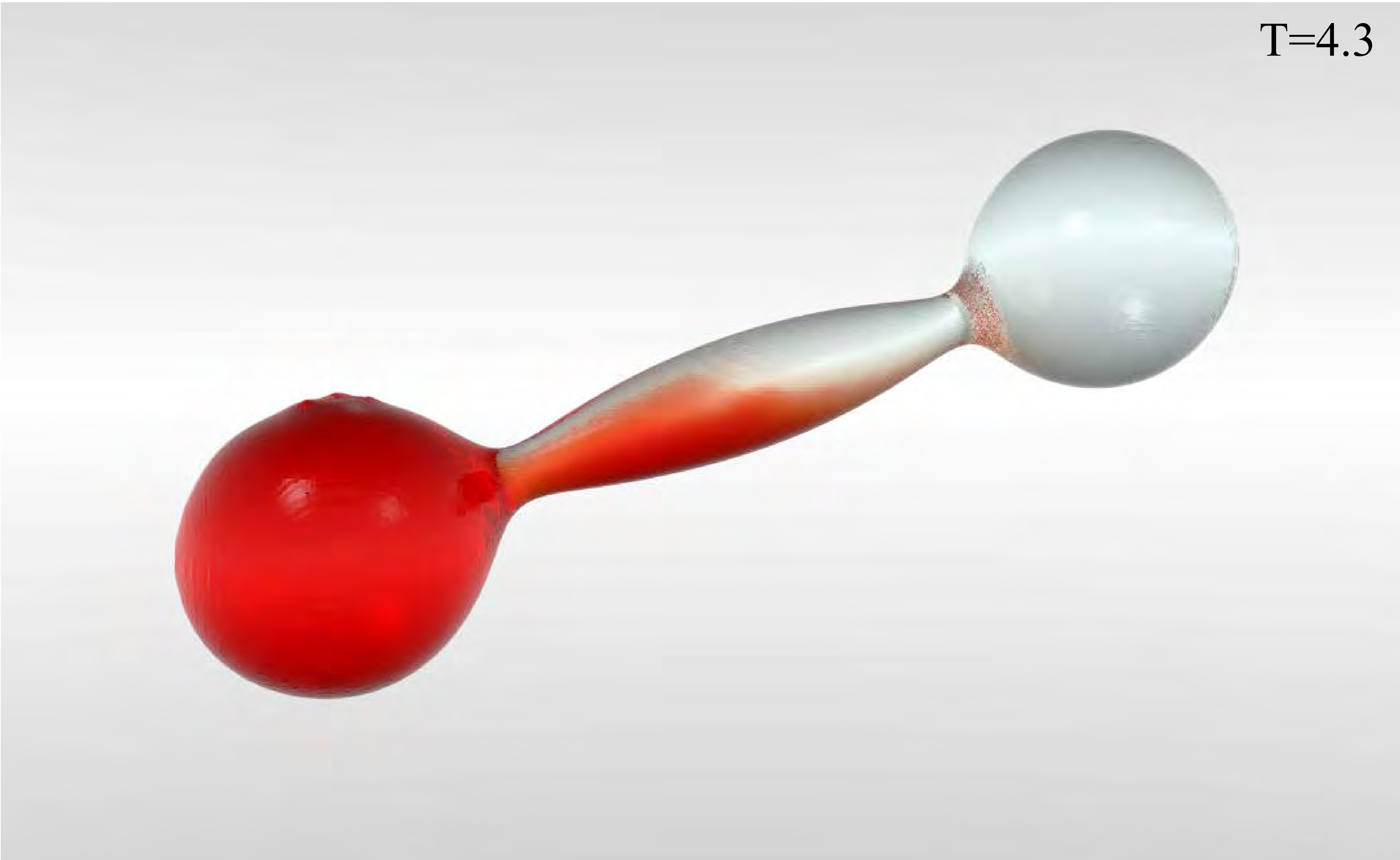

T=1.4

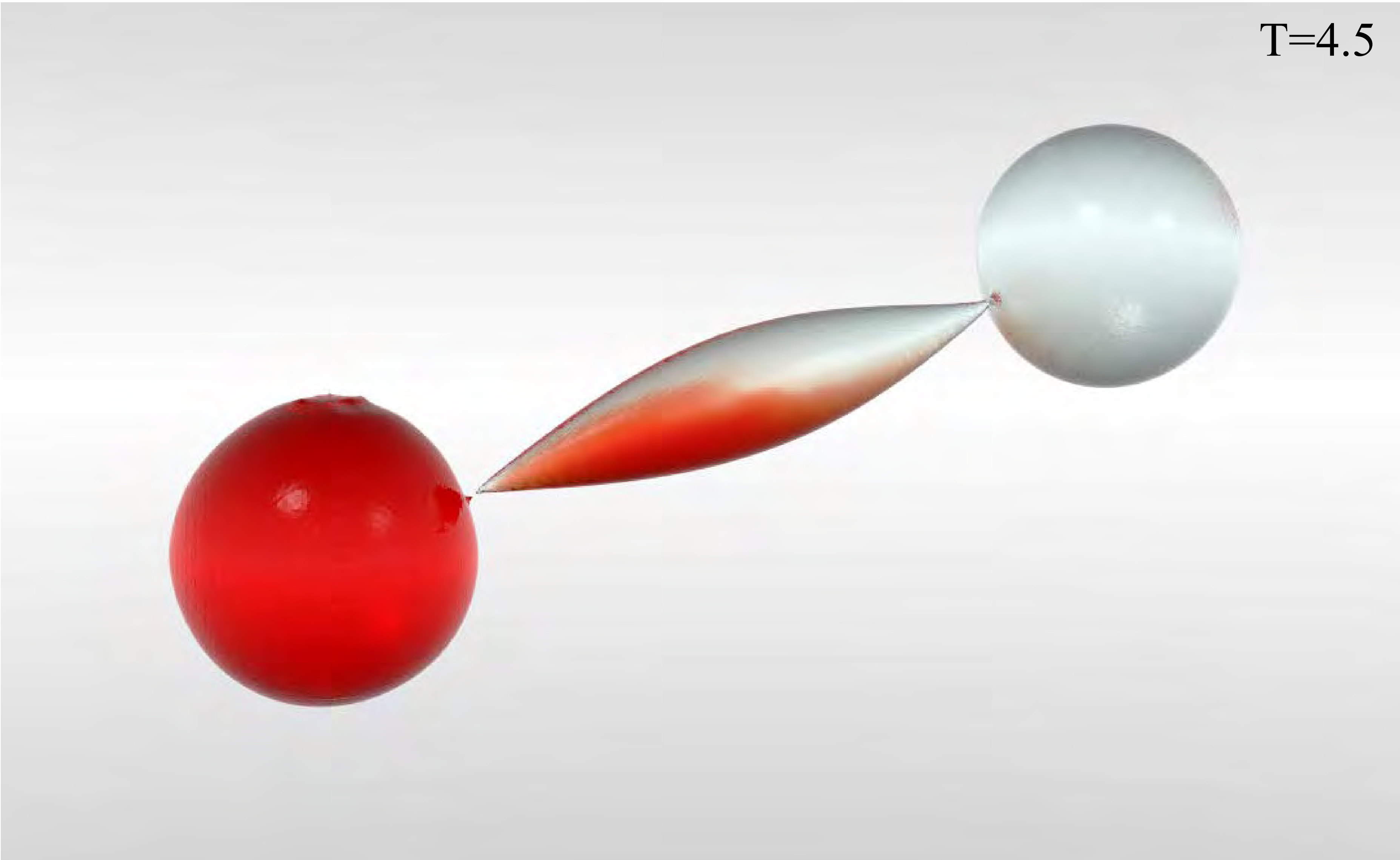

T=1.6

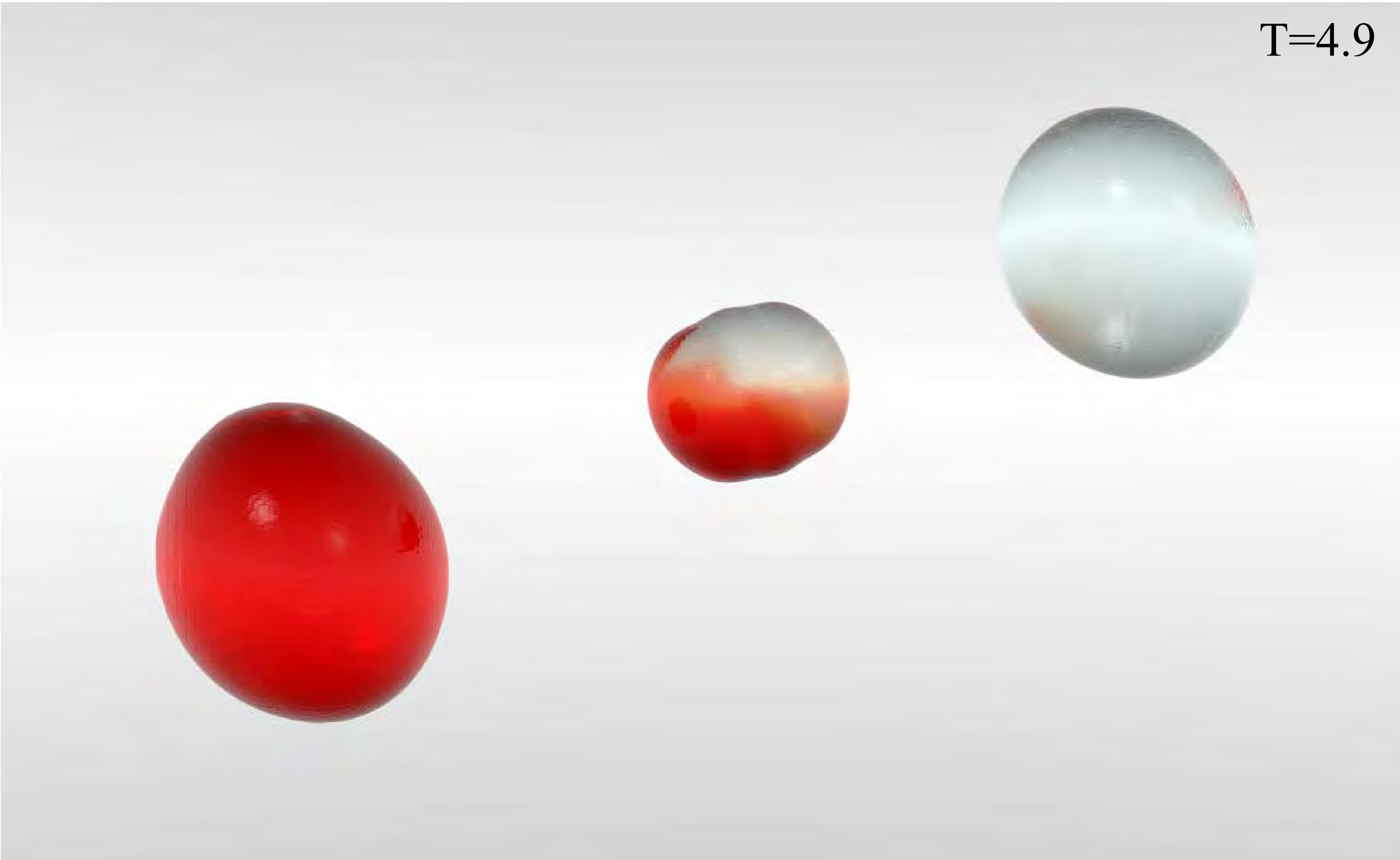
T=1.9

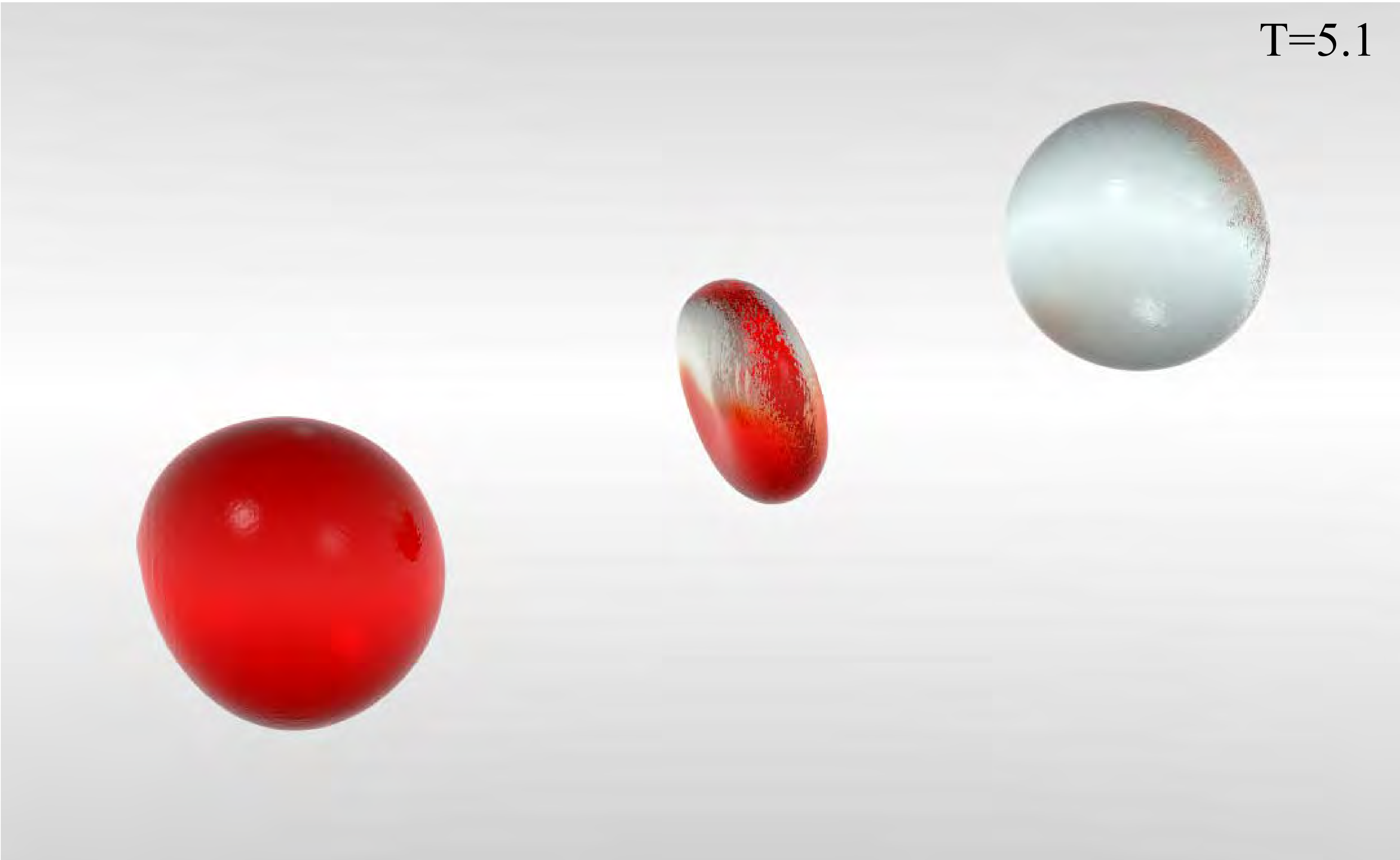

T=2.1

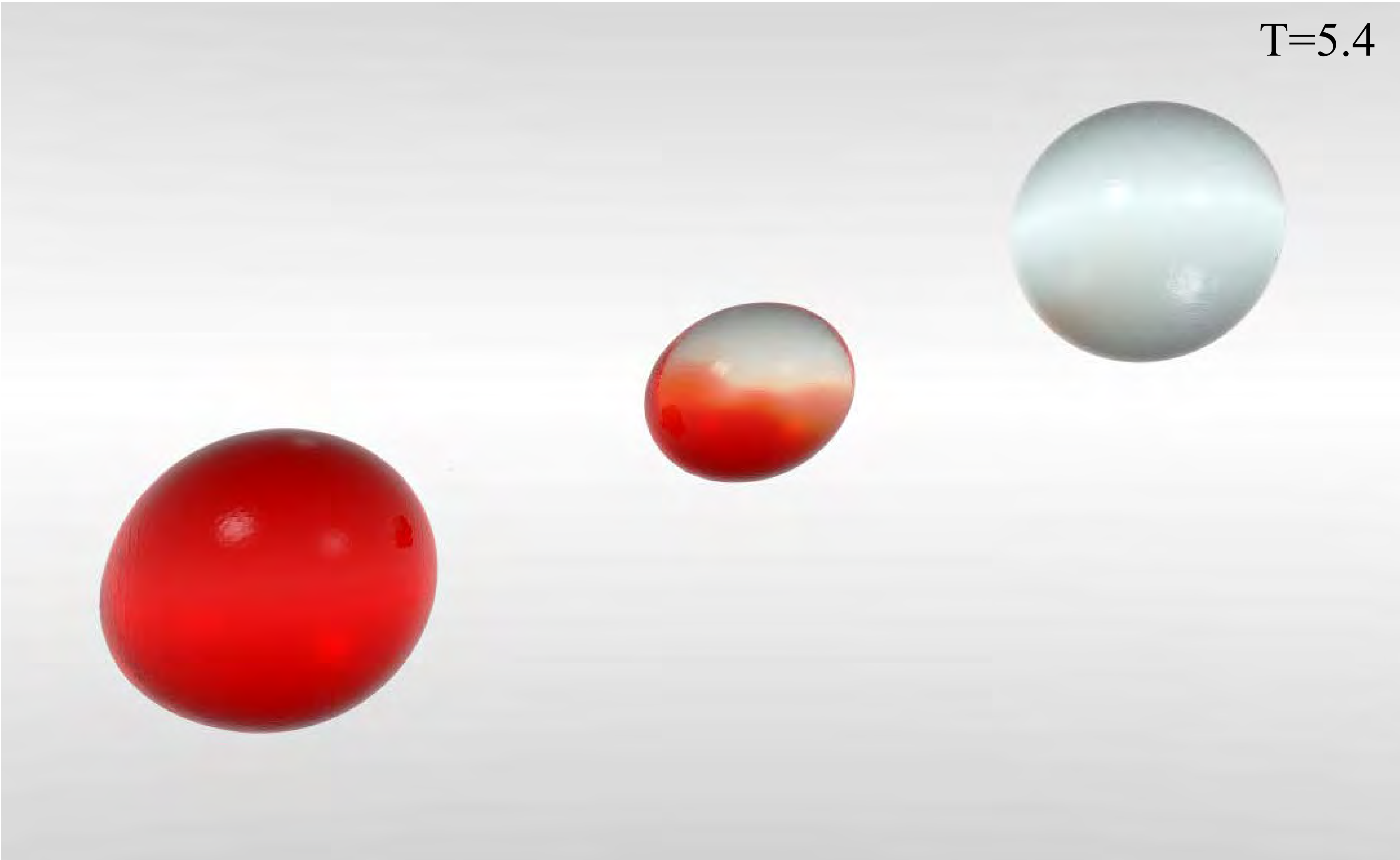

T=2.9


T=4.3

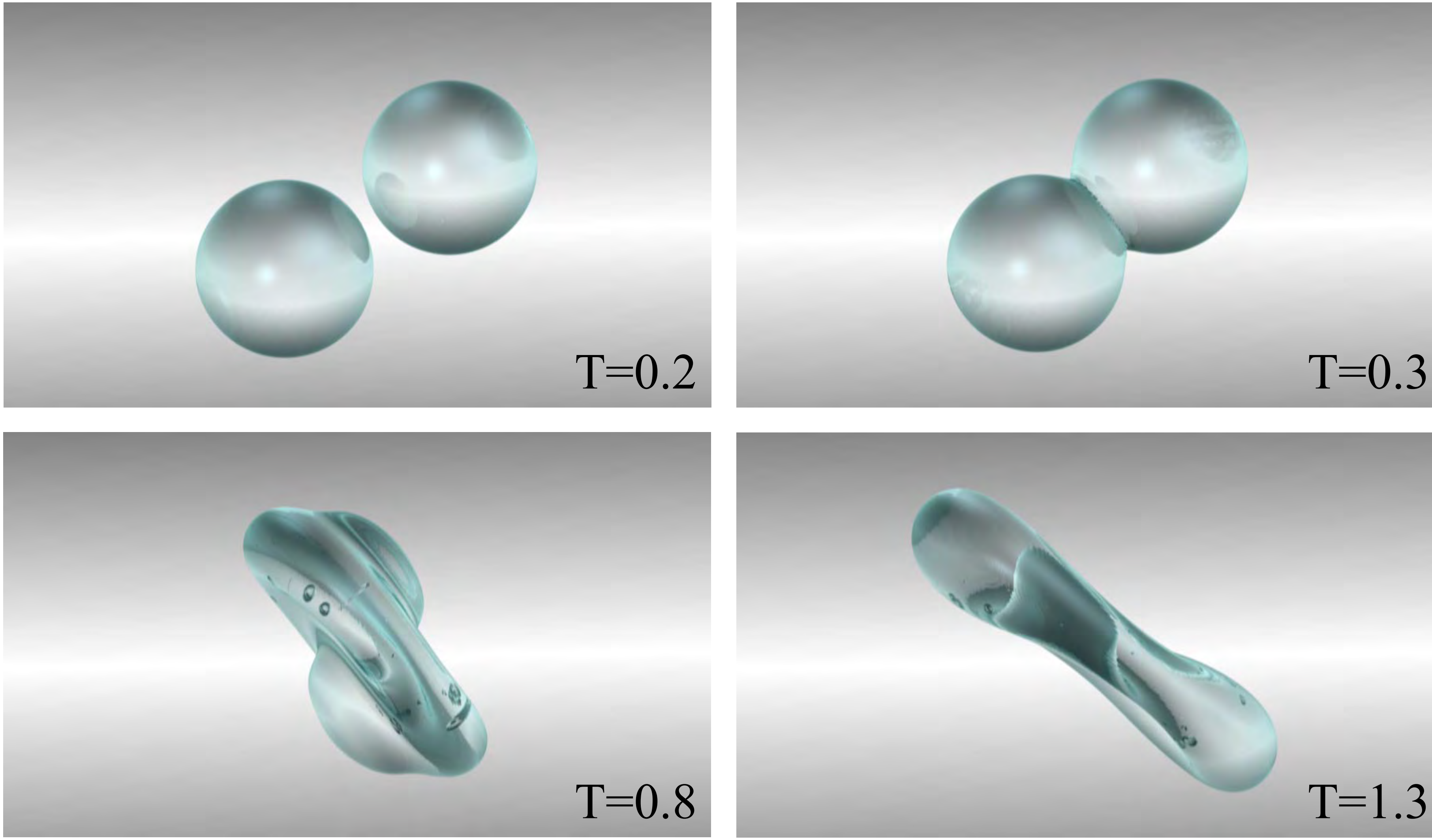

T=4.5


T=4.9

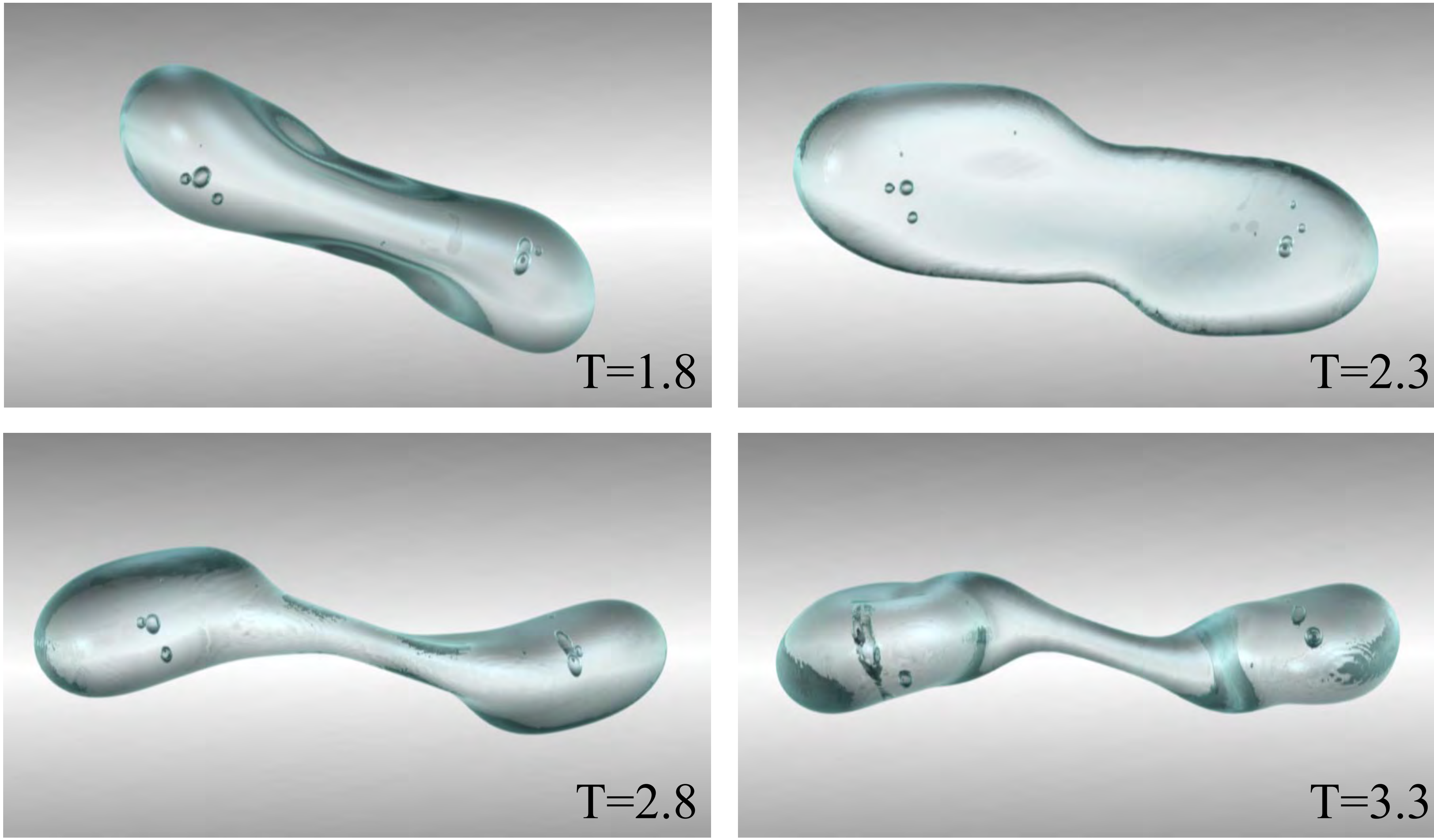

T=5.1

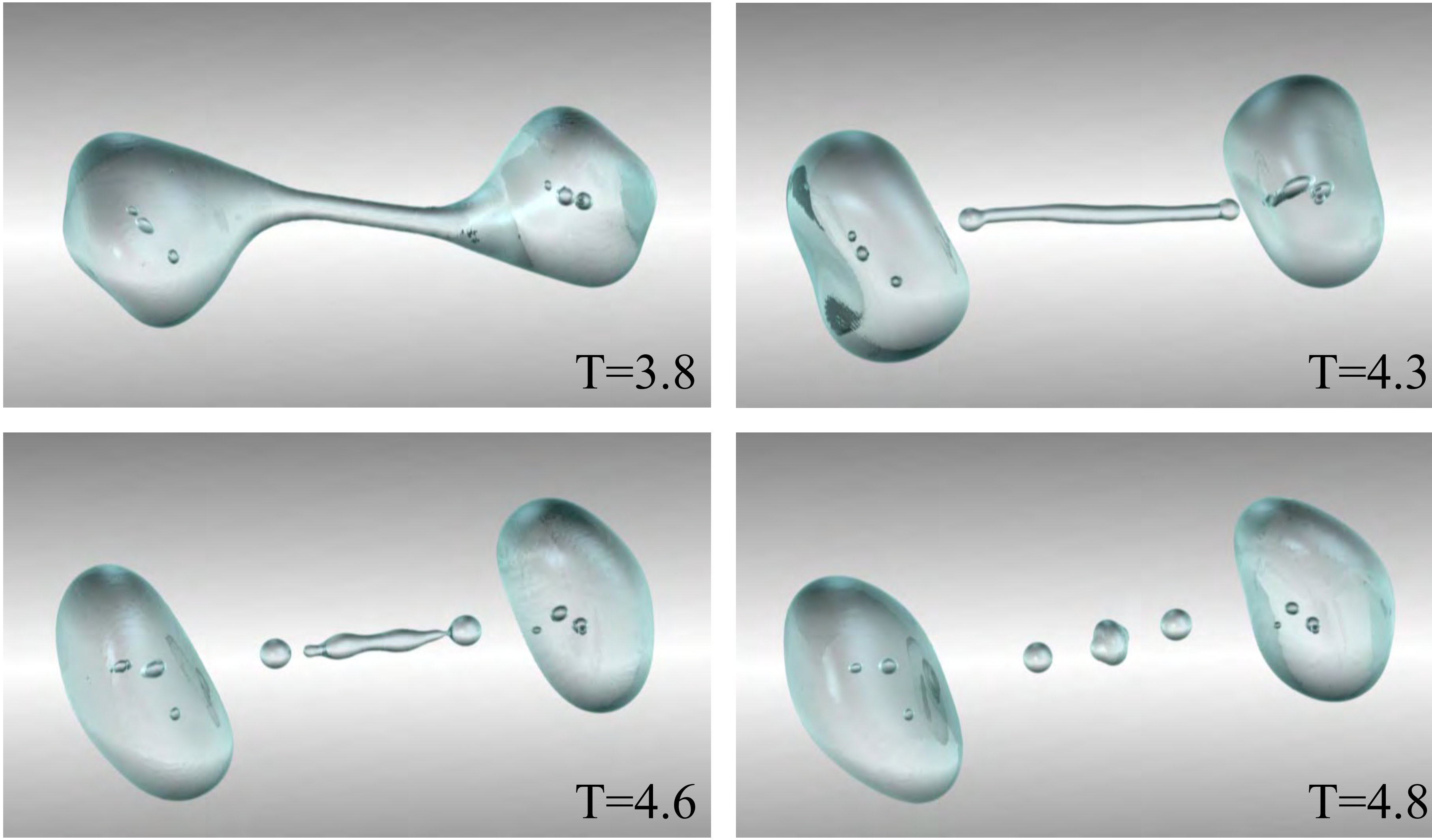

T=5.4

Droplet Collision & Stretching Separation



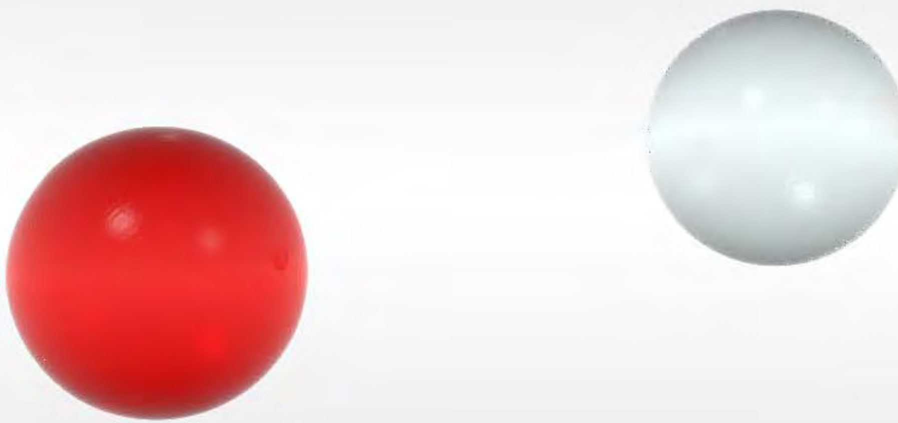
We=65.1, Re=320.3, B=0.49, D=370 μm, U=2.43 m/s, ρ=758 kg/m^3, μ= 2.13$\times 10^{-3}$ N·s/m^2

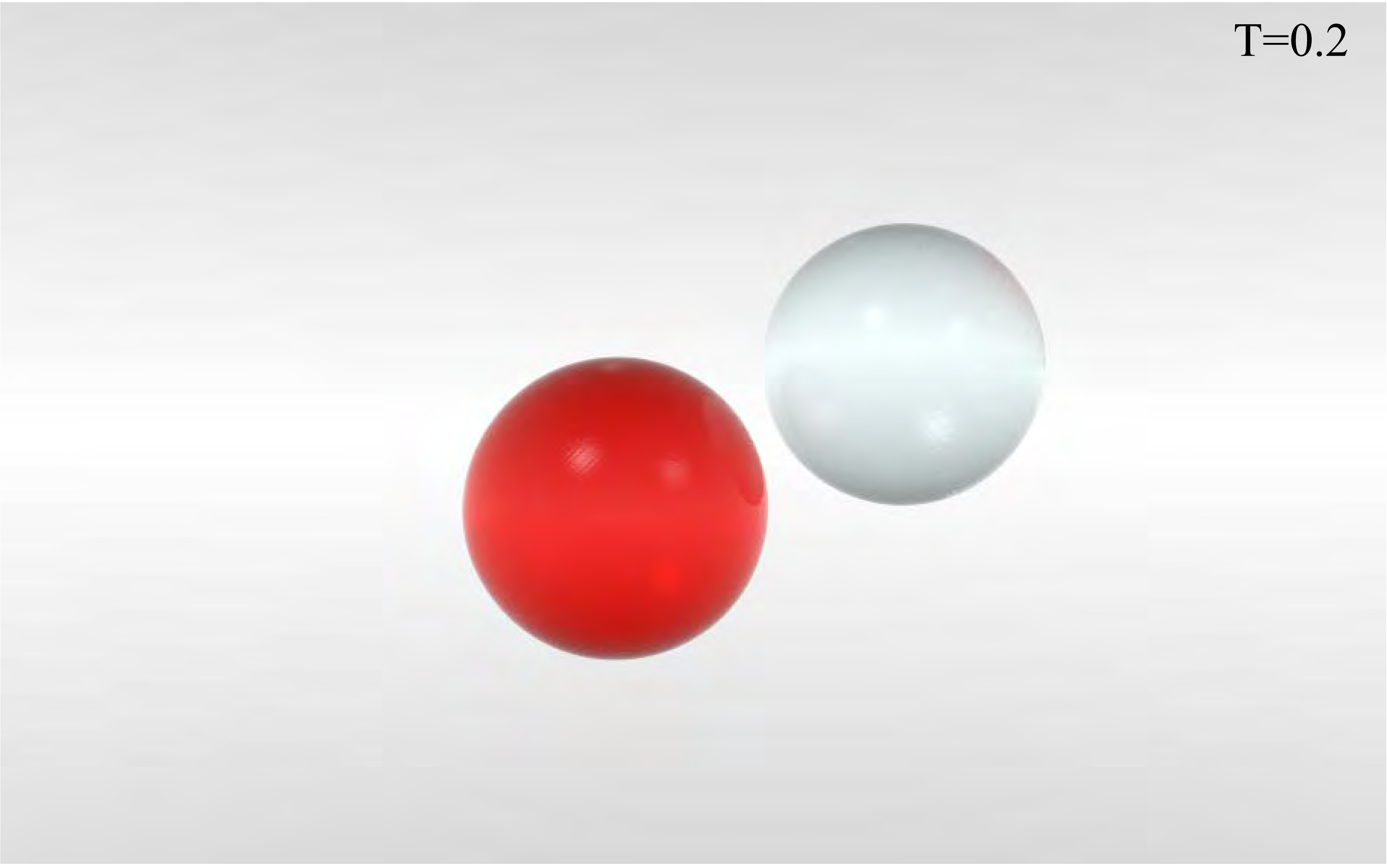

T=1.8
T=2.3
T=2.8
T=3.3

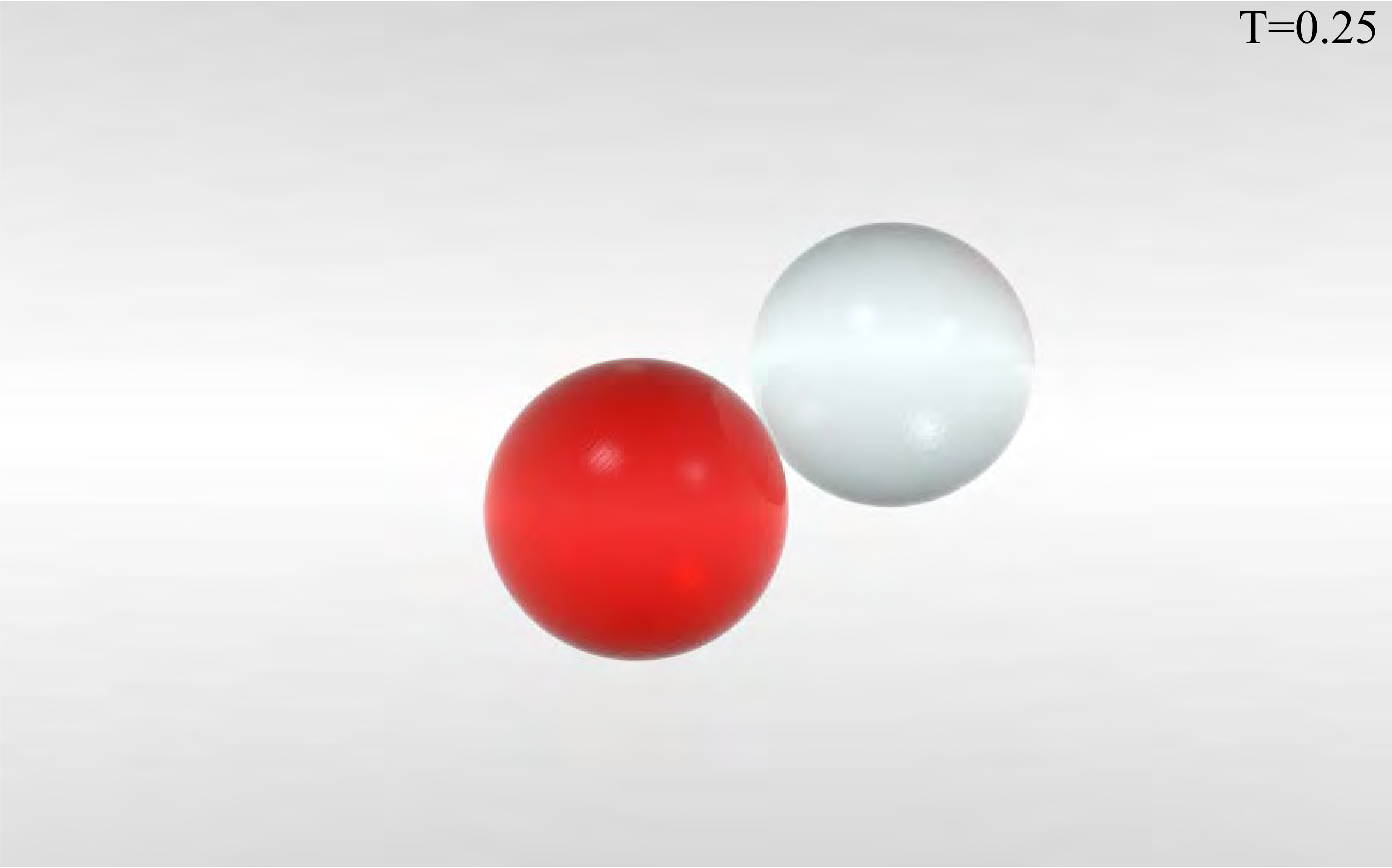

T=3.8
T=4.3
T=4.6
T=4.8

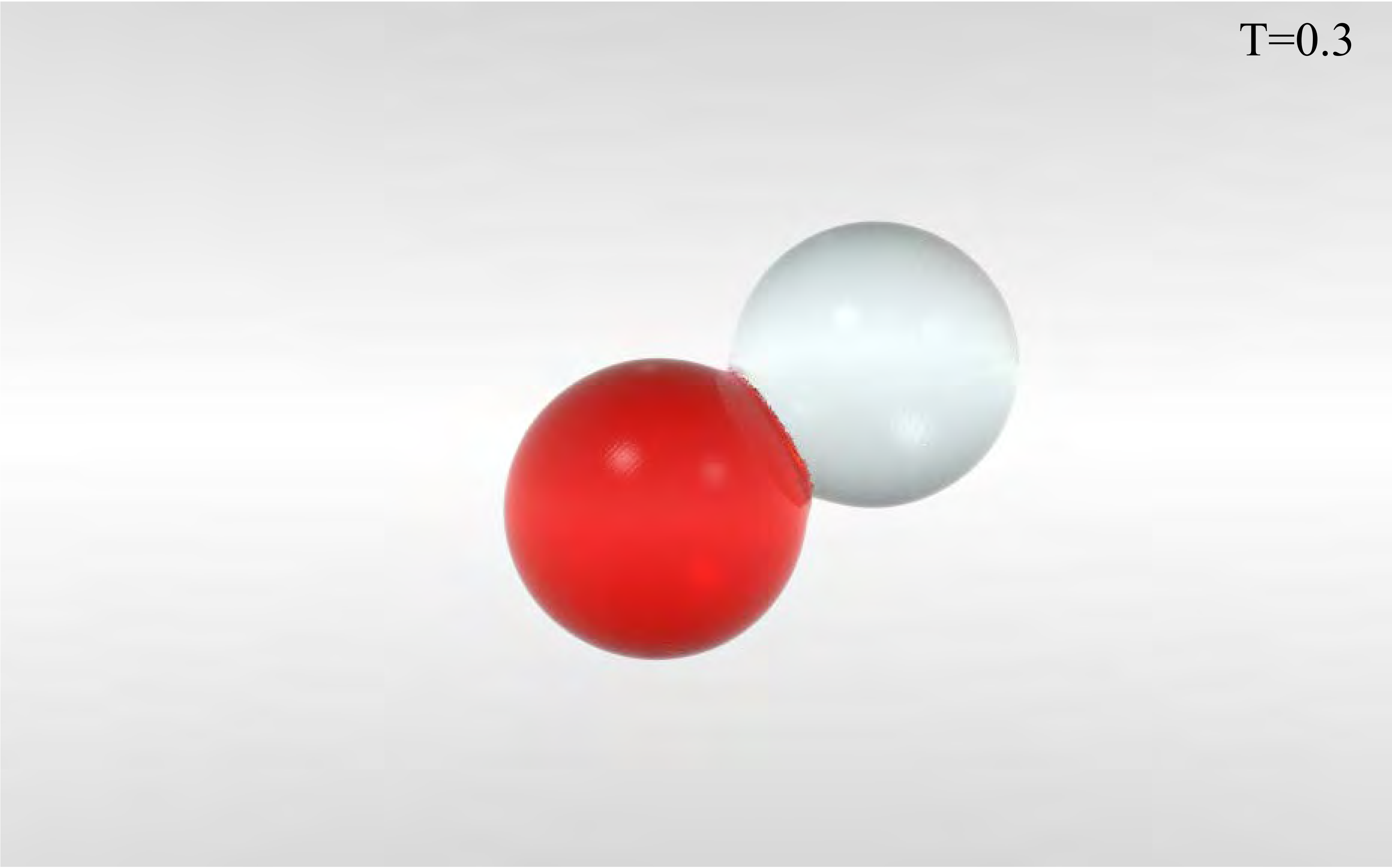
Droplet Collision & Stretching Separation

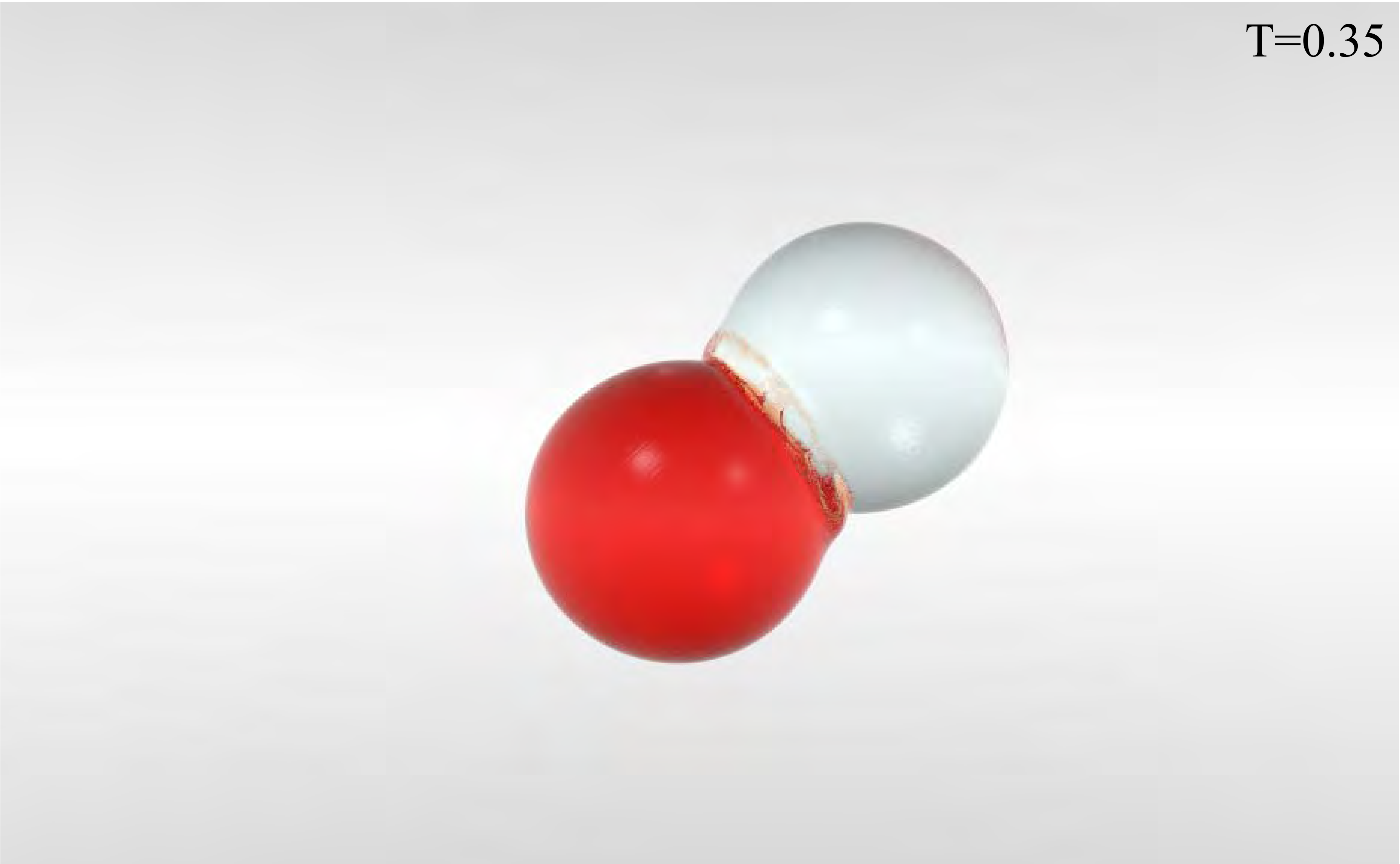
Movie




T=0.2


T=0.25


T=0.3


T=0.35

T=0.4


T=0.45

T=0.5

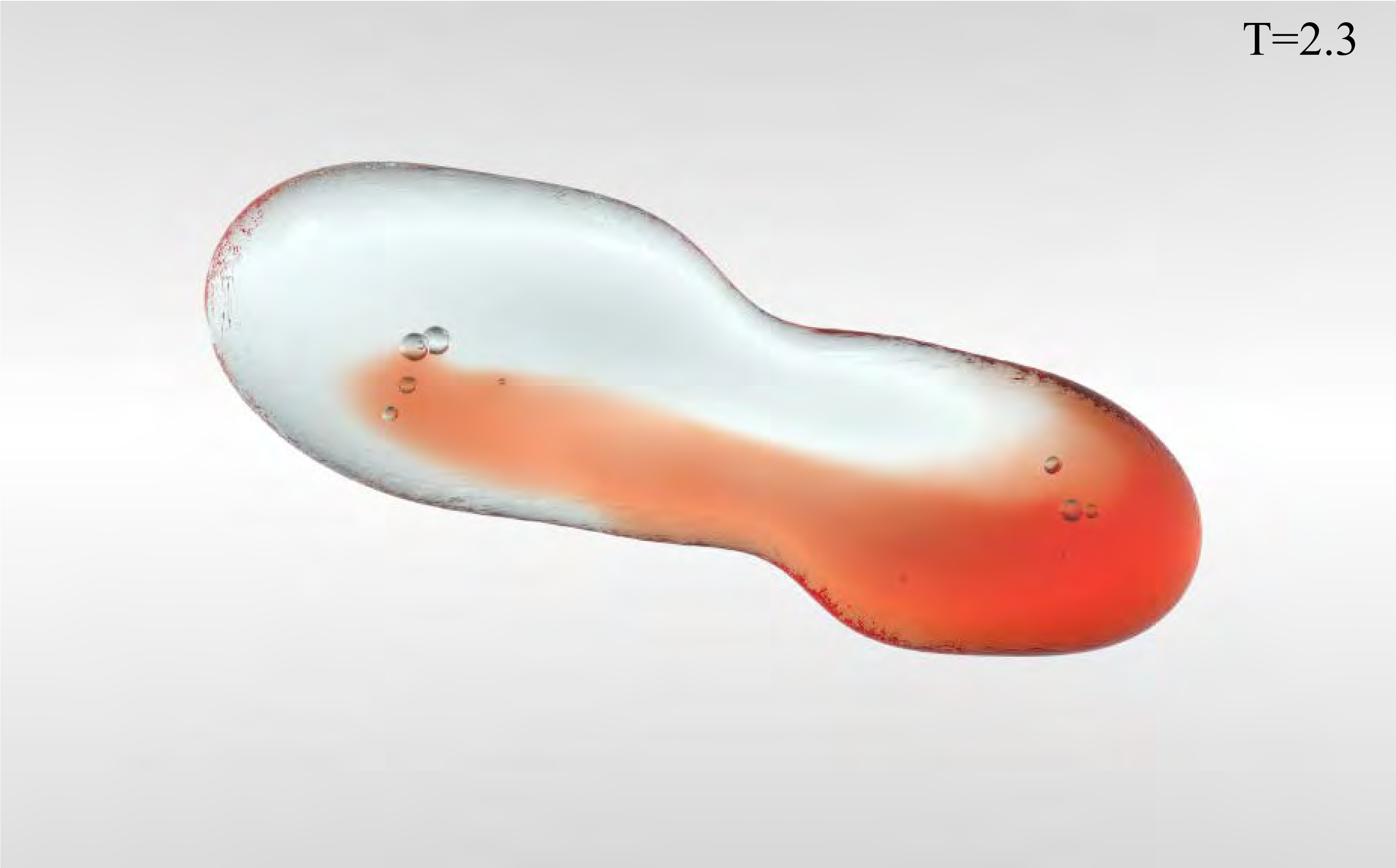

T=0.55


T=0.6


T=0.8

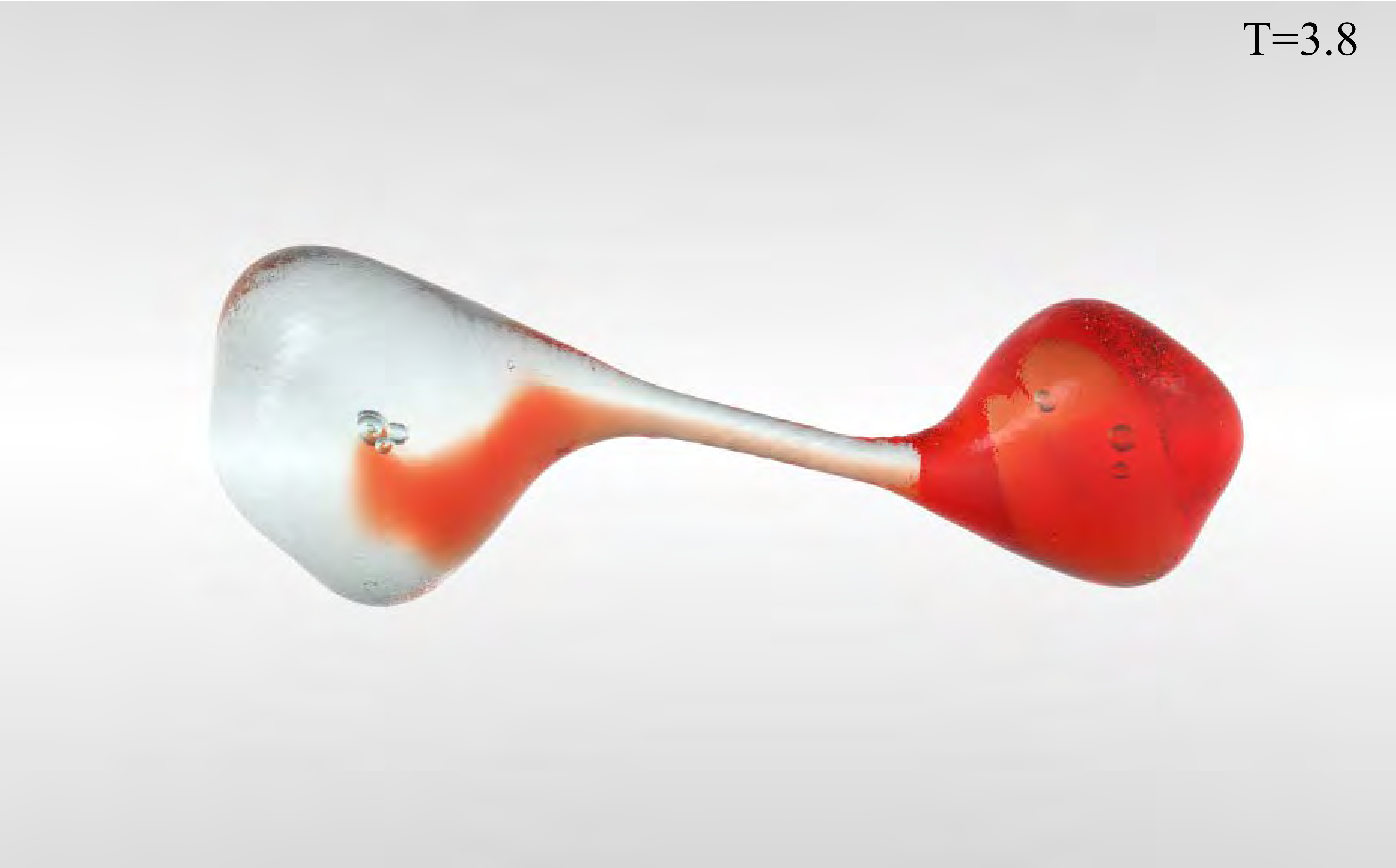

T=1.3

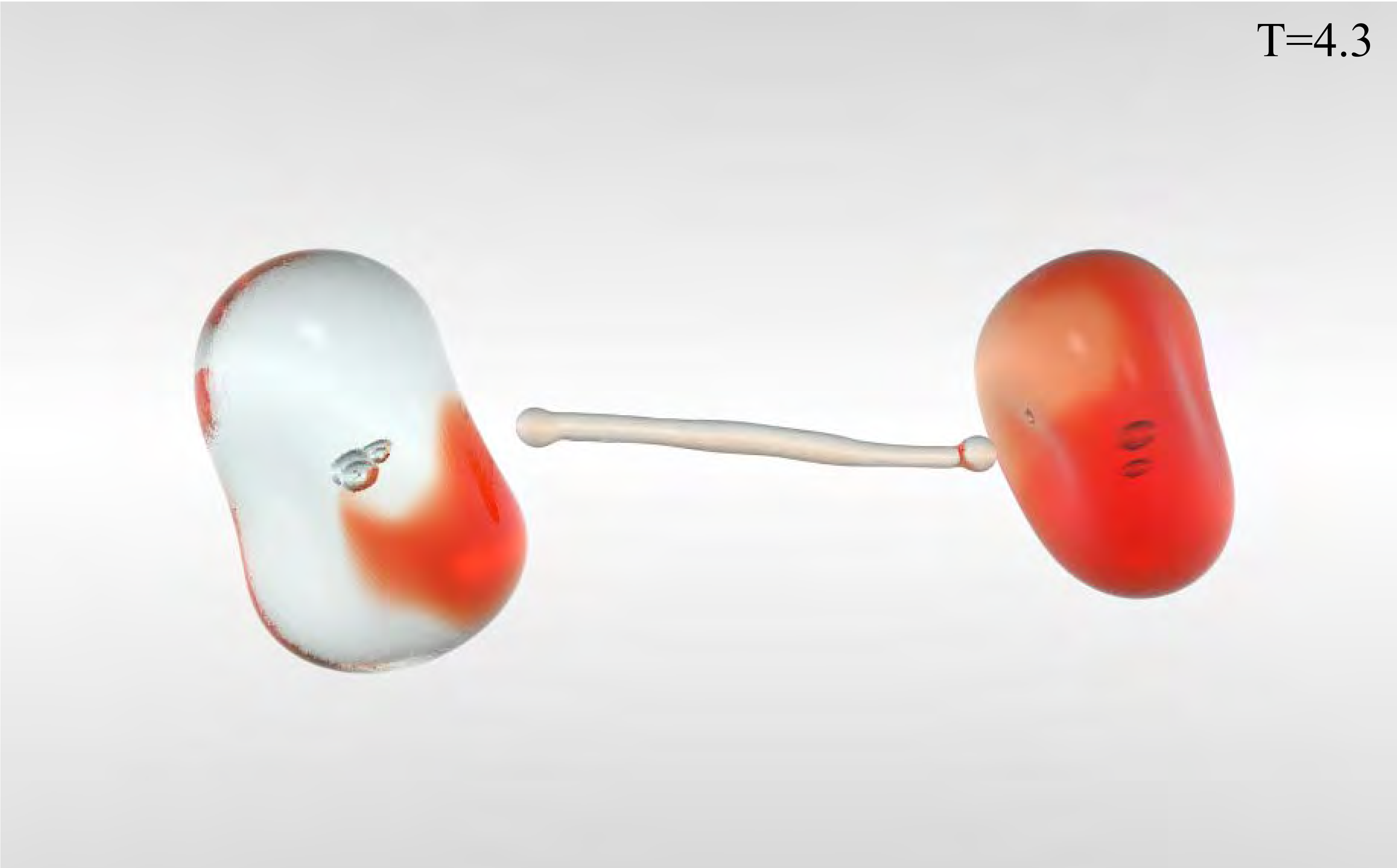

T=1.8

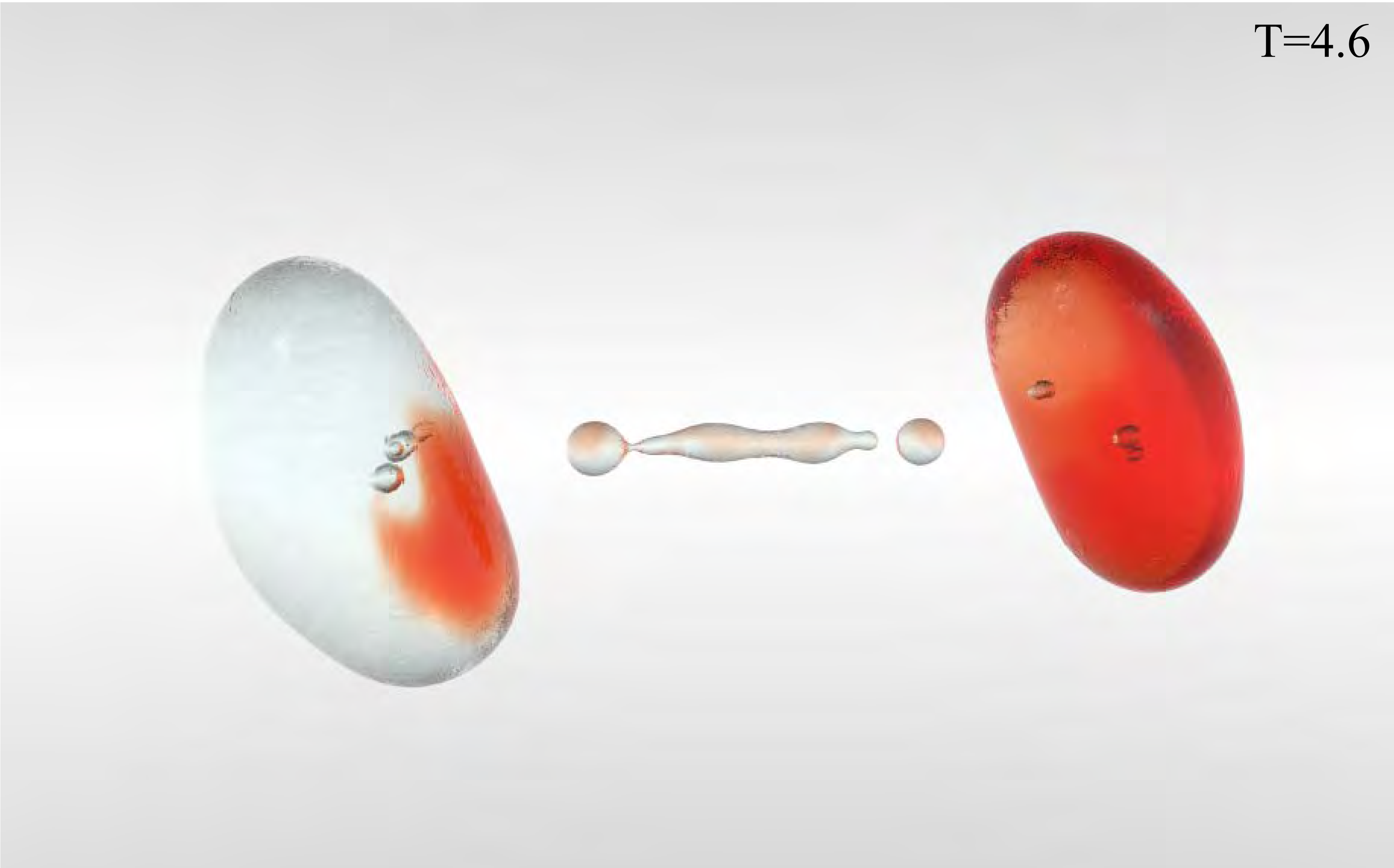

T=2.3

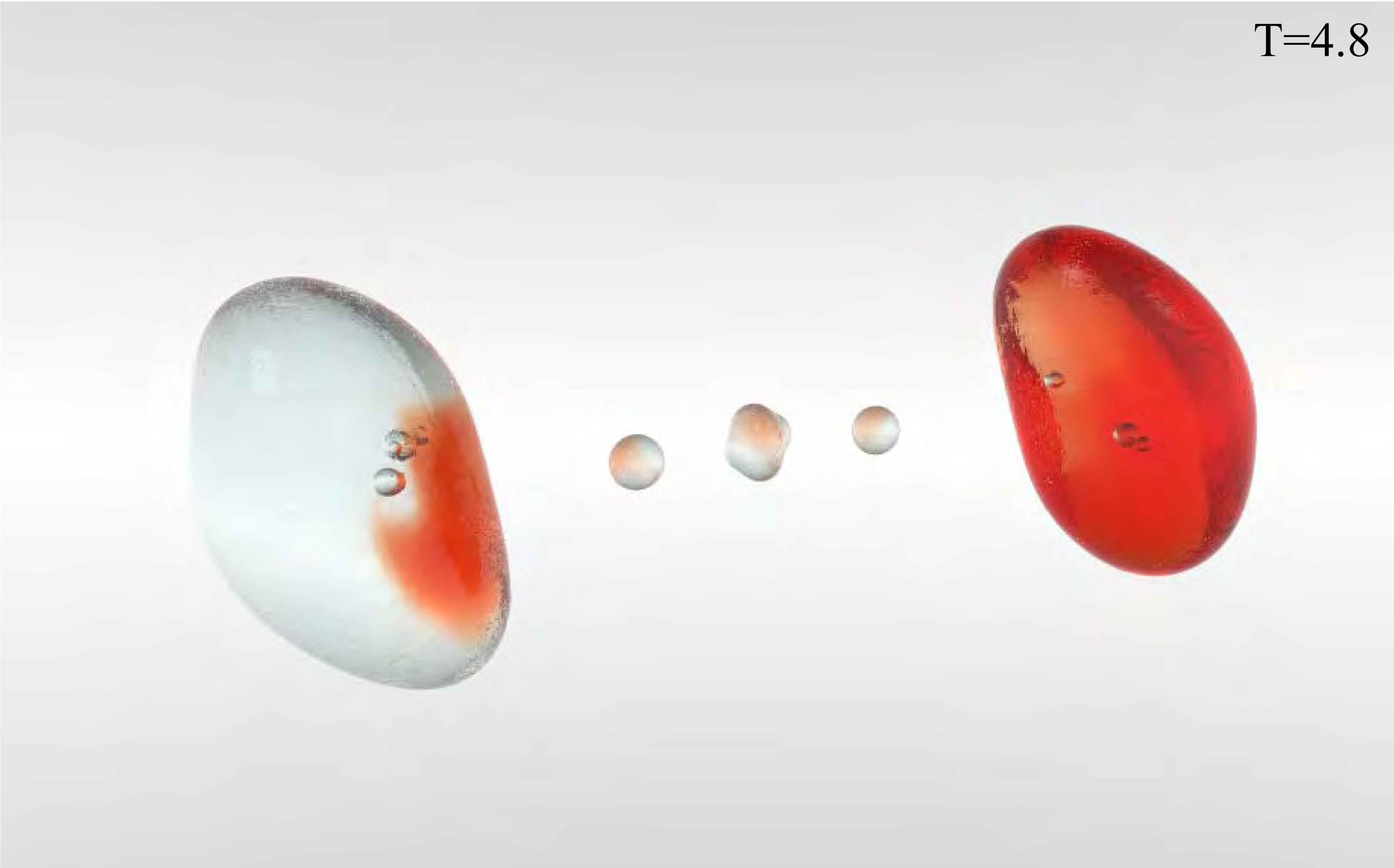

T=2.8

T=3.3


T=3.8


T=4.3


T=4.6


T=4.8

Droplet Collision Dynamics and Mixing

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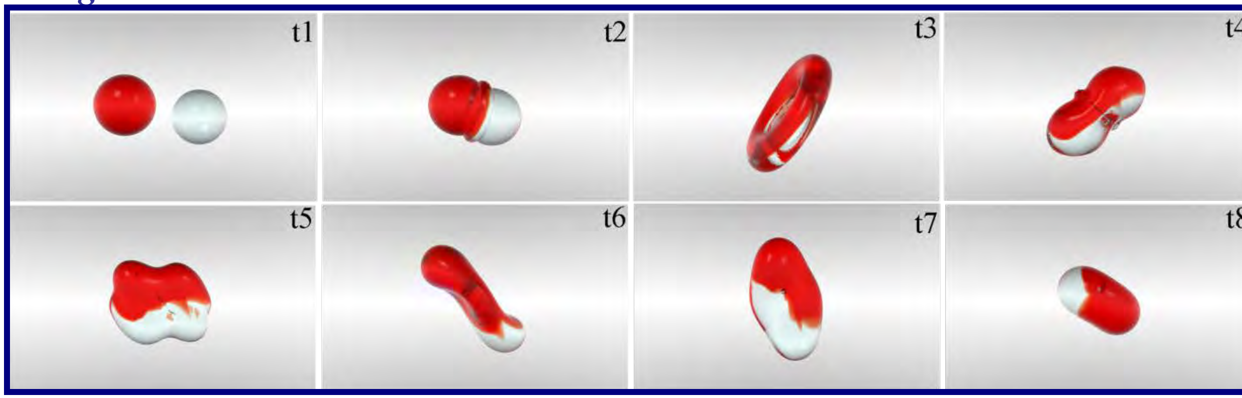
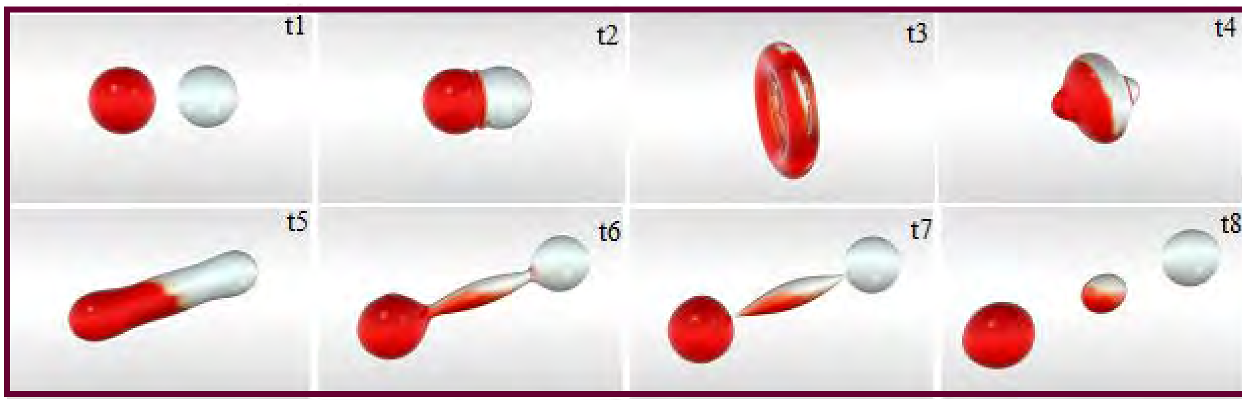
Coalescence

We=60, Re=292.9, B=0.2
D=336 μm, U=2.45m/s.



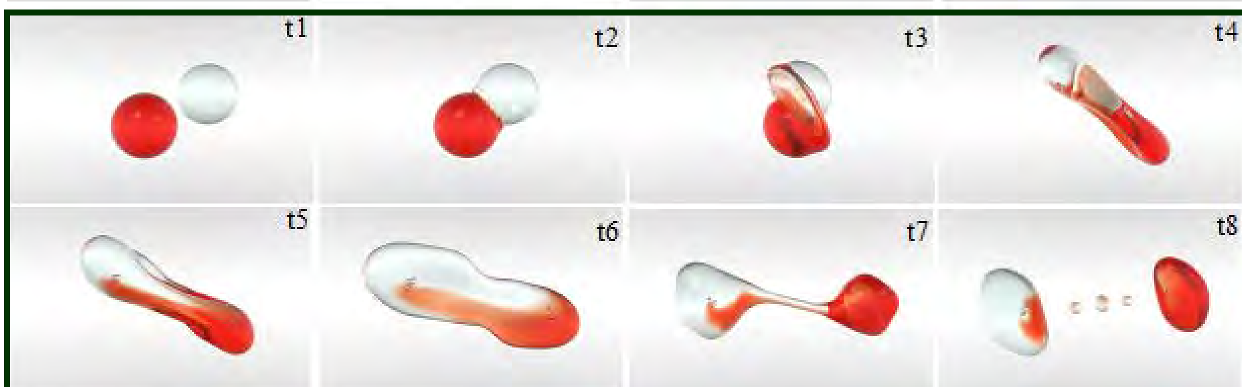
Reflexive Separation

We=61.4, Re=296.5, B=0.06
D=336 μm, U=2.48 m/s.

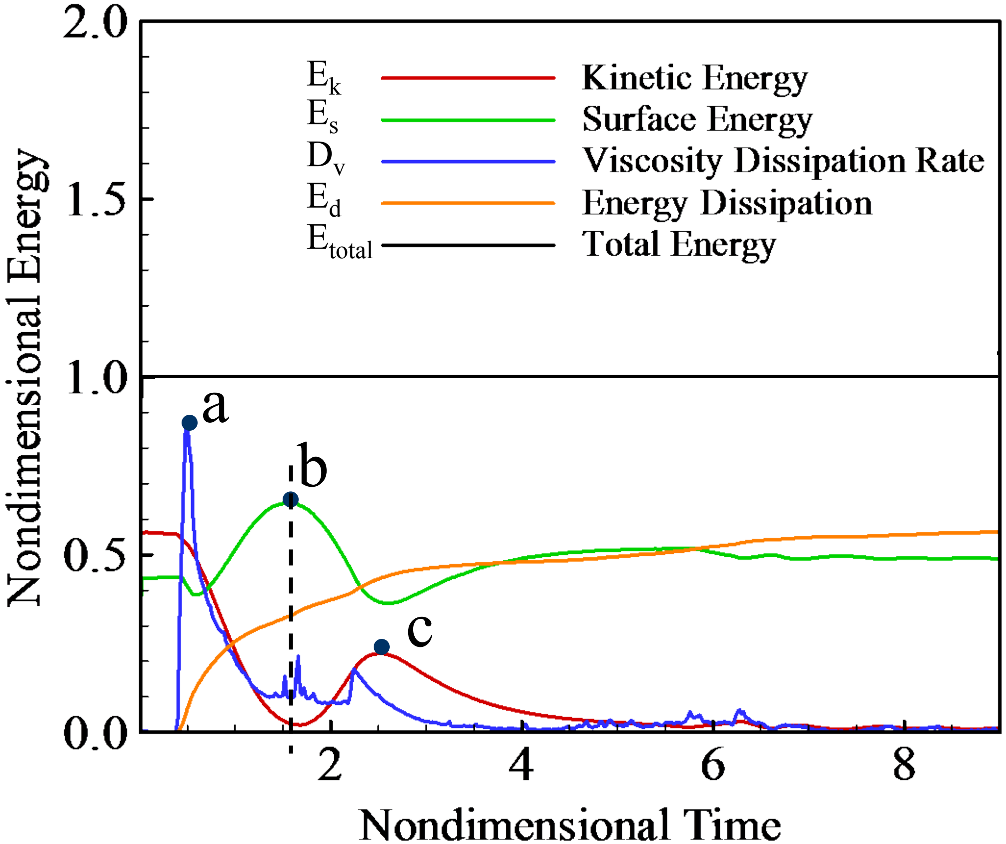


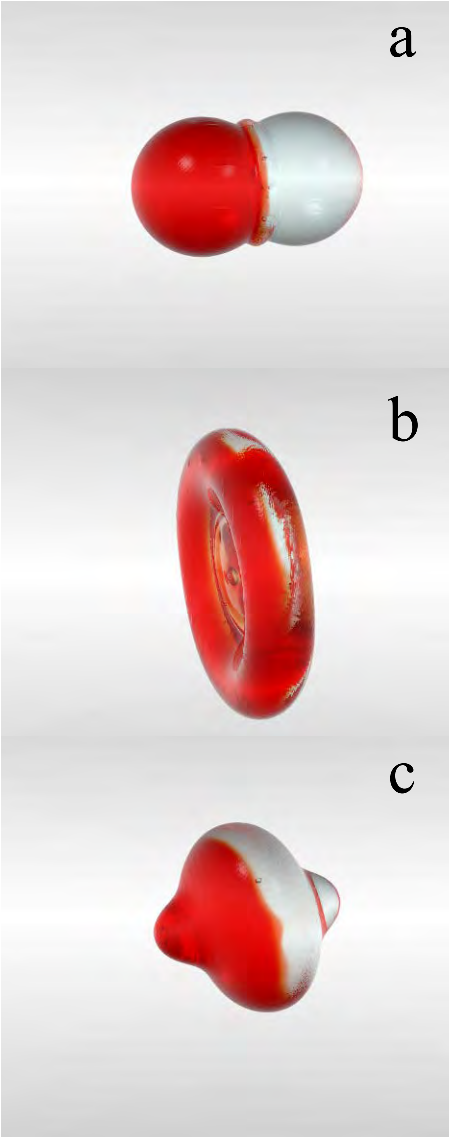
Stretching Separation

We=65.1, Re=320.3, B=0.49
D=370 μm, U=2.43 m/s.



Energy Budget & Droplet Shape





$$E_k = \int_0^{V_{all}} \frac{1}{2}\rho U^2 \mathrm{d}V \qquad E_s = \sigma S \qquad E_d = \int_0^t \int_0^{V_{all}} \Phi \mathrm{d}V \mathrm{d}t$$

$$E_{total} = E_k + E_s + E_d$$

Contour of Mass Transfer Rate

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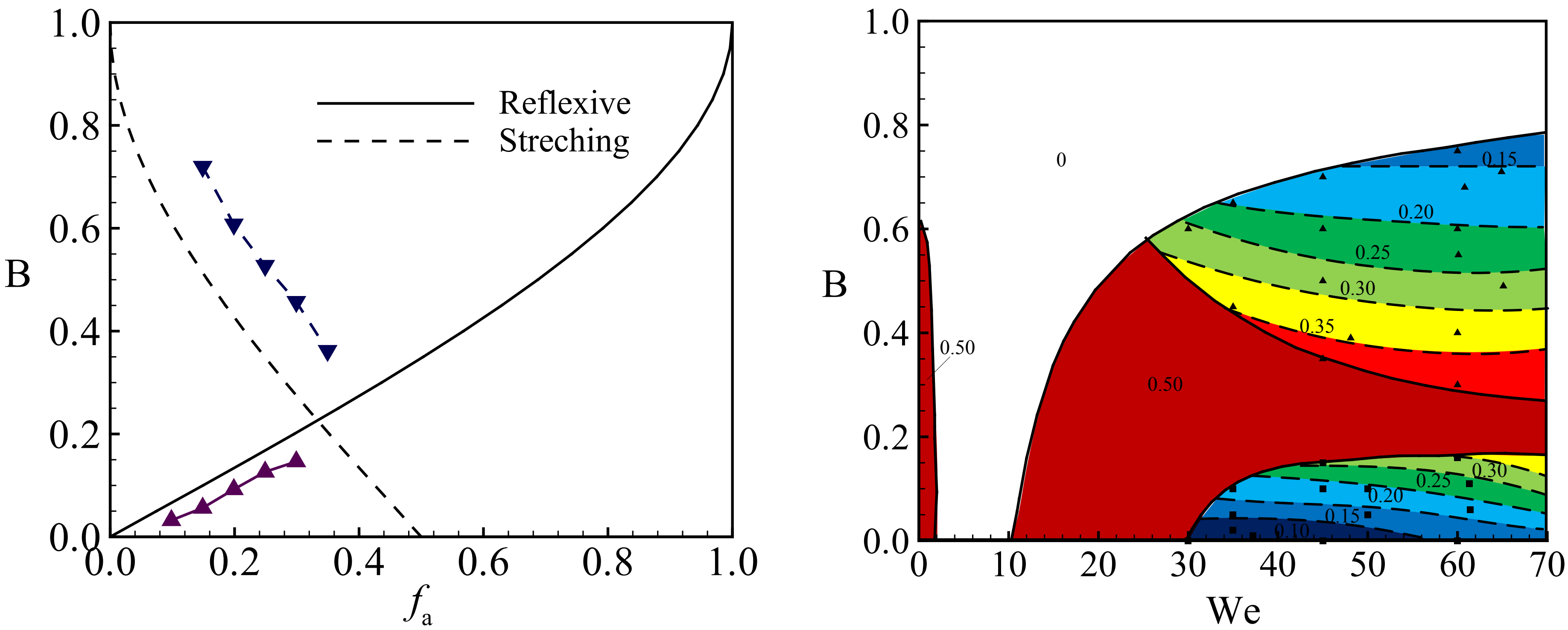
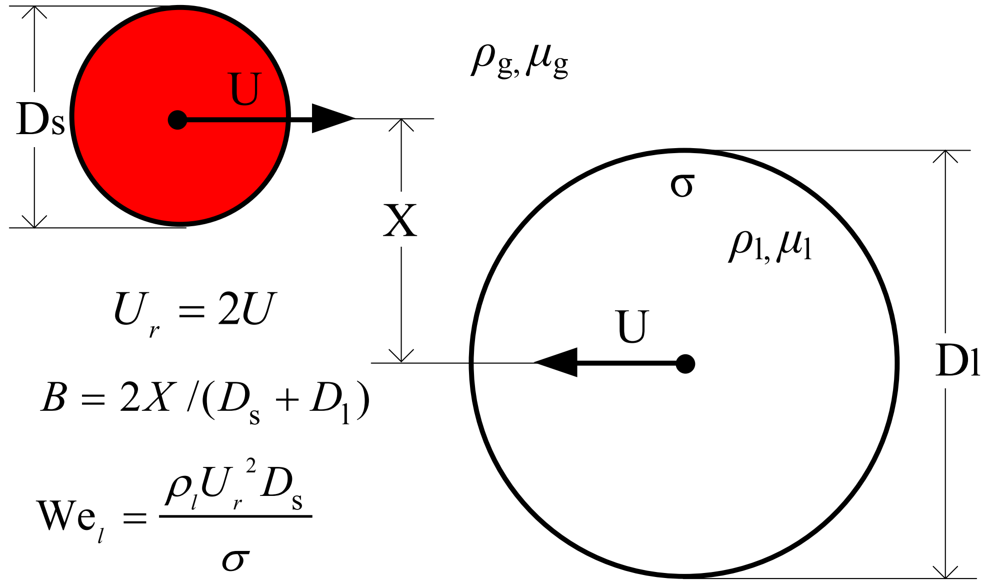


- Without considering practical effects, such as shear layer mixing, the model gives some agreement with the simulation results;
- The practical effect can be introduced into present model by adding empirical constant.

Unequal-sized Droplet Collision

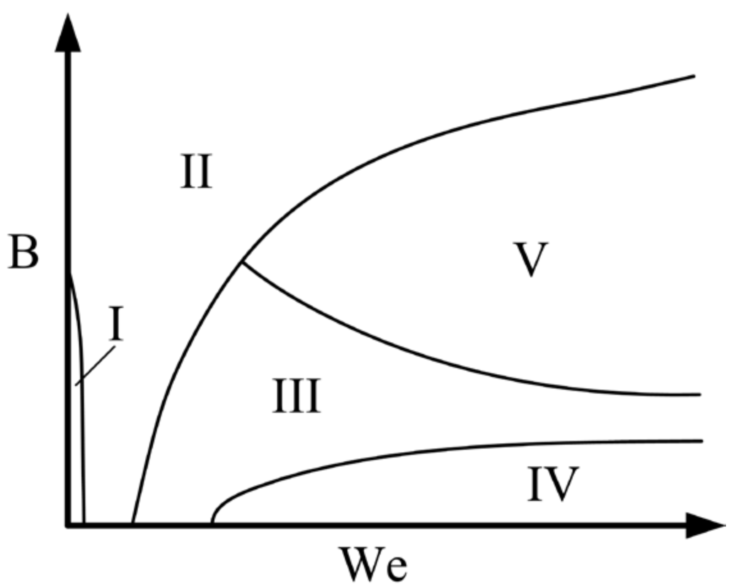
water in 1 atm air
density ratio: 815
viscosity ratio: 56



$$U_r = 2U$$

$$B = 2X/(D_s + D_l)$$

$$\mathrm{We}_l = \frac{\rho_l U_r^2 D_s}{\sigma}$$



I. coalescence after minor deformation
II. bouncing
III. coalescence after major deformation
IV. reflexive separation
V. stretching separation

Unequal Reflexive Separation

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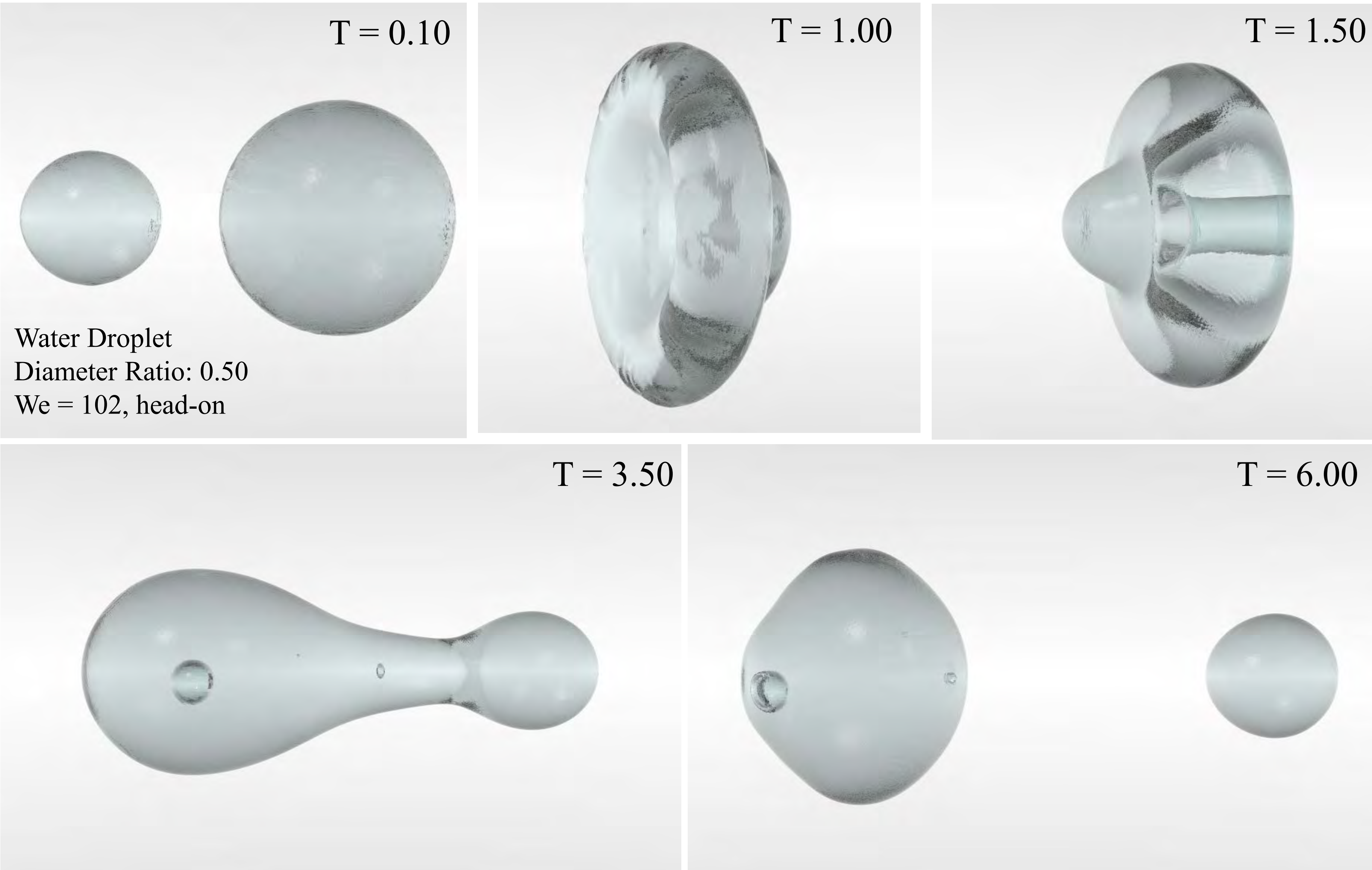
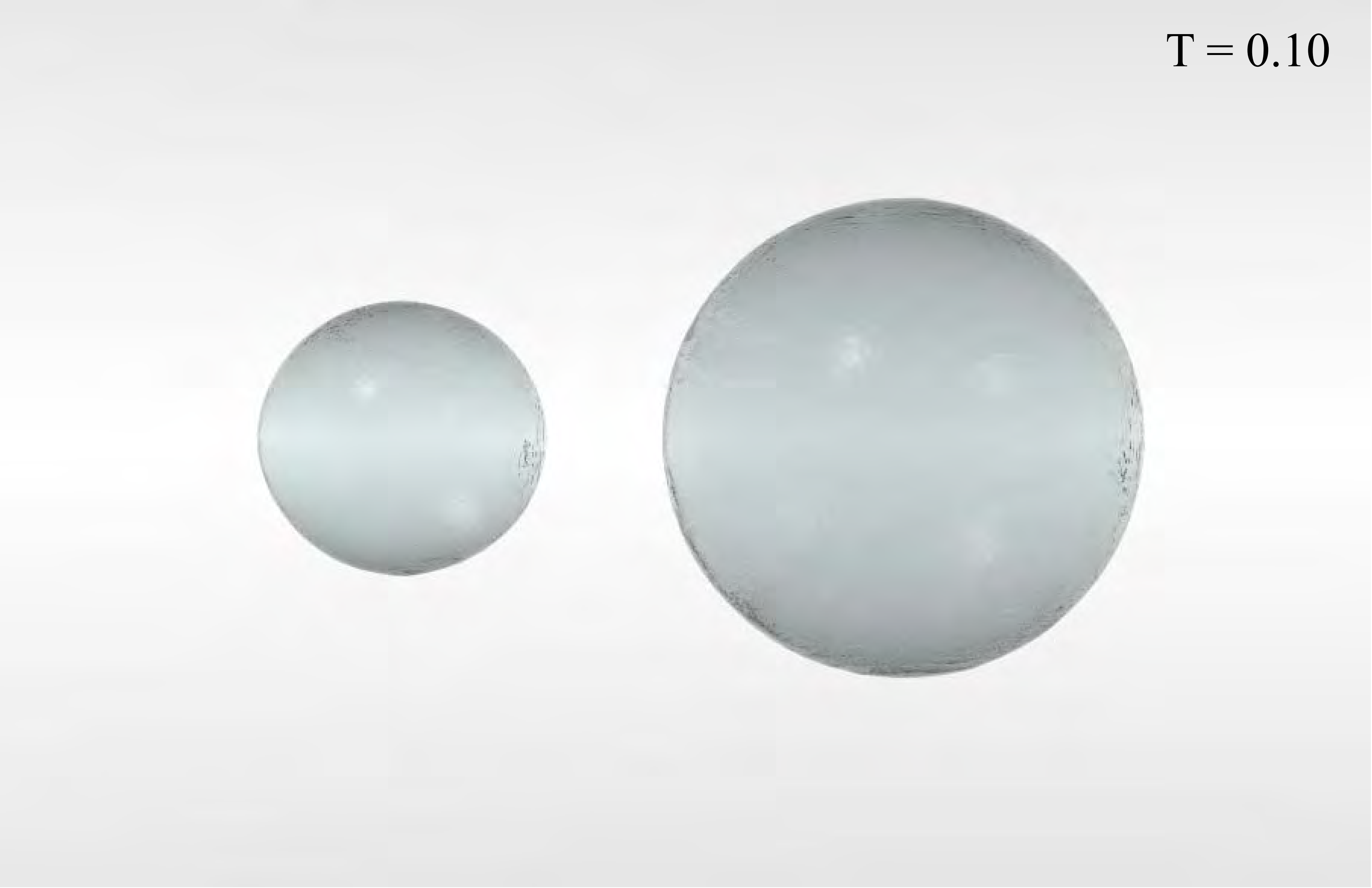
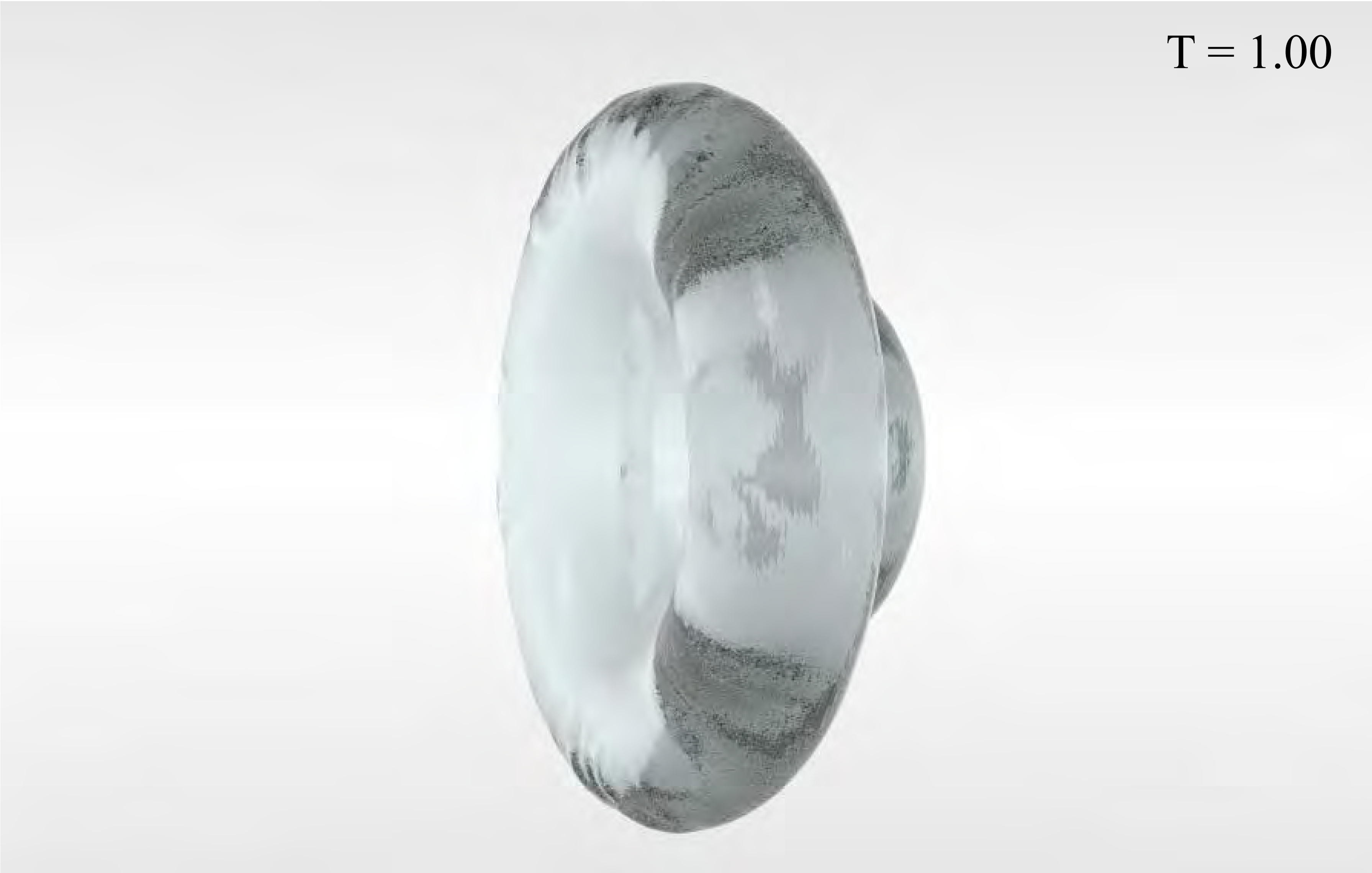


Unequal Reflexive Separation
Droplet Diameter Ratio: 0.50



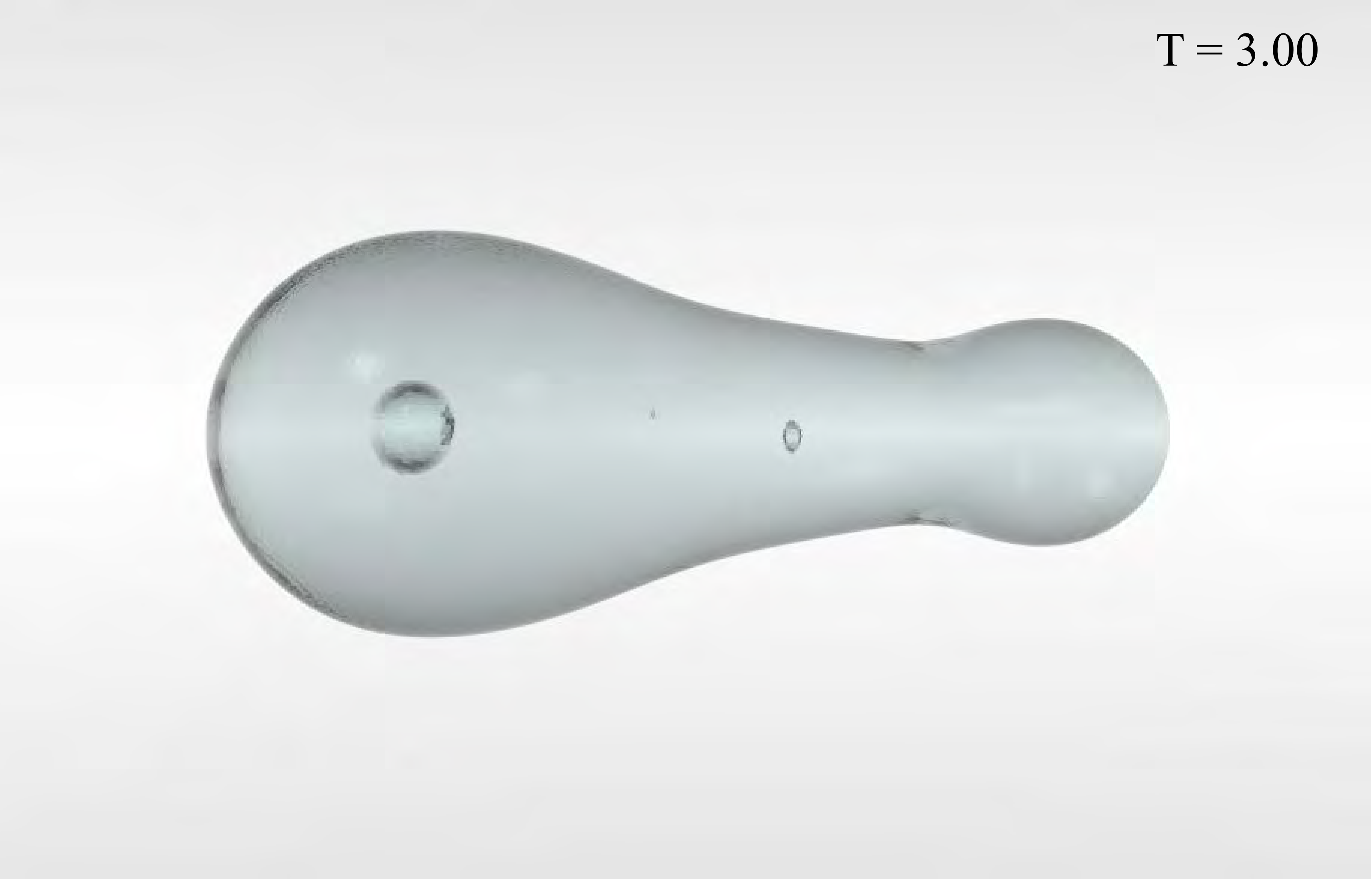

T = 0.50

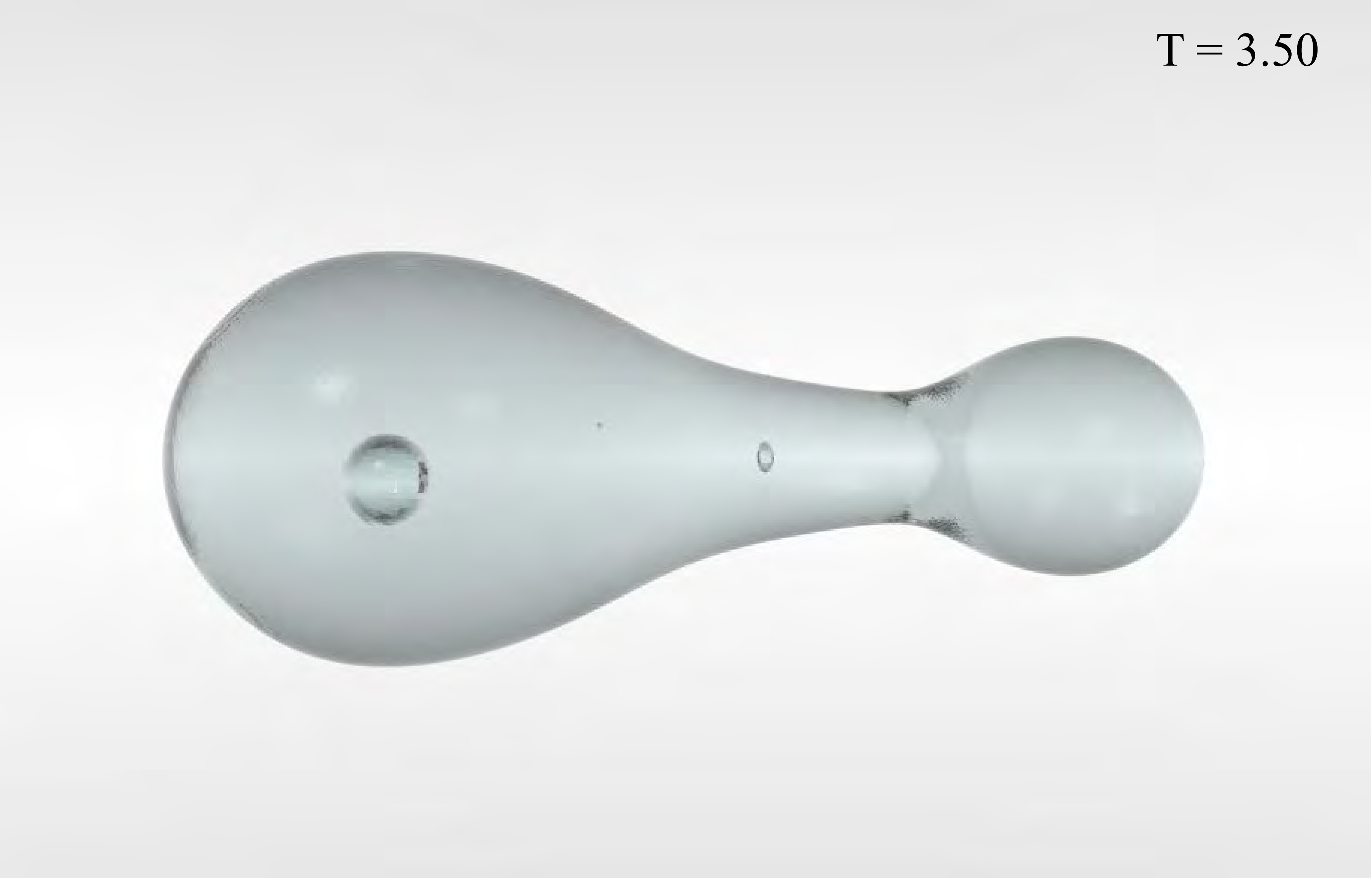

T = 1.00

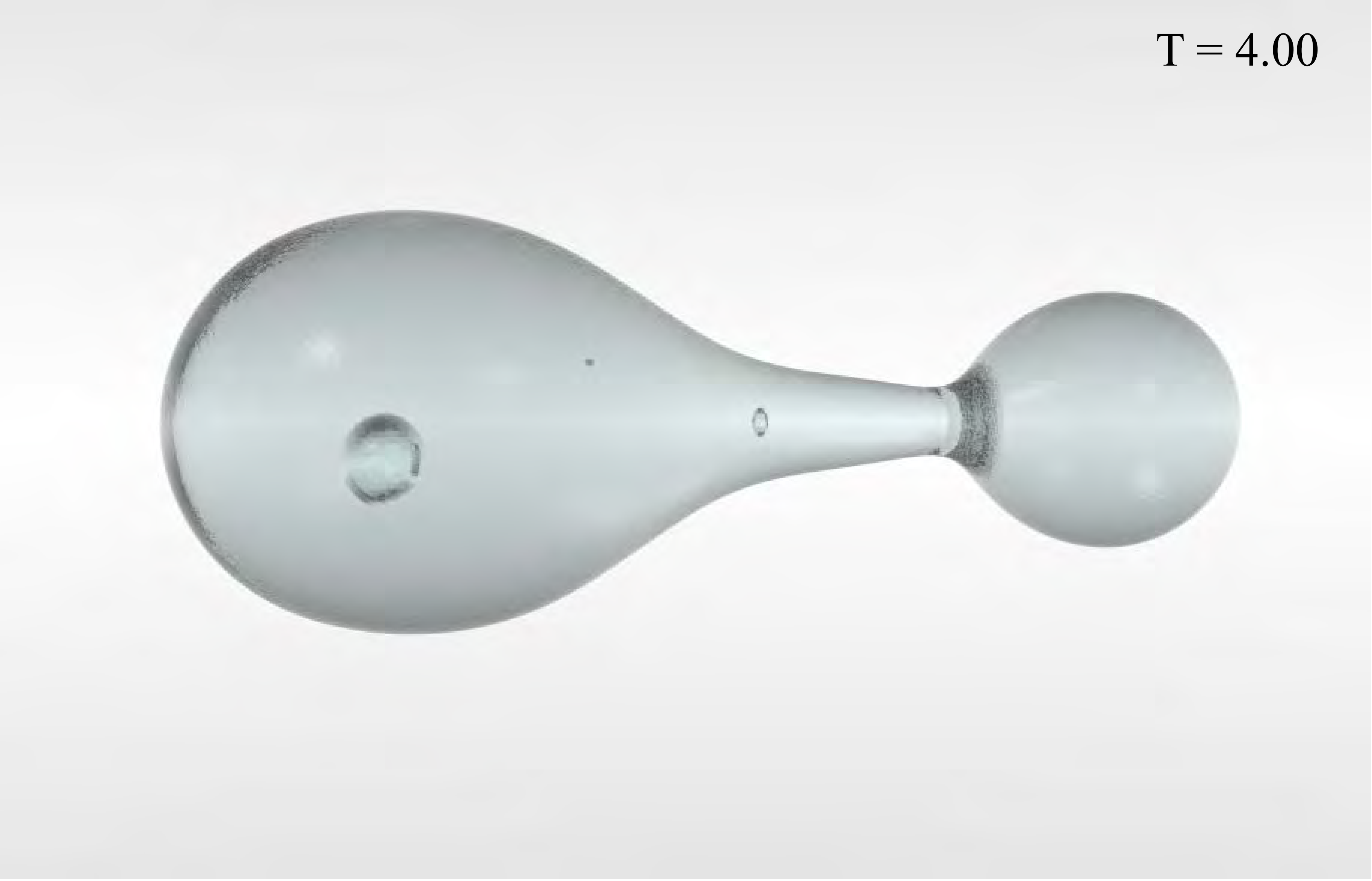
T = 1.50

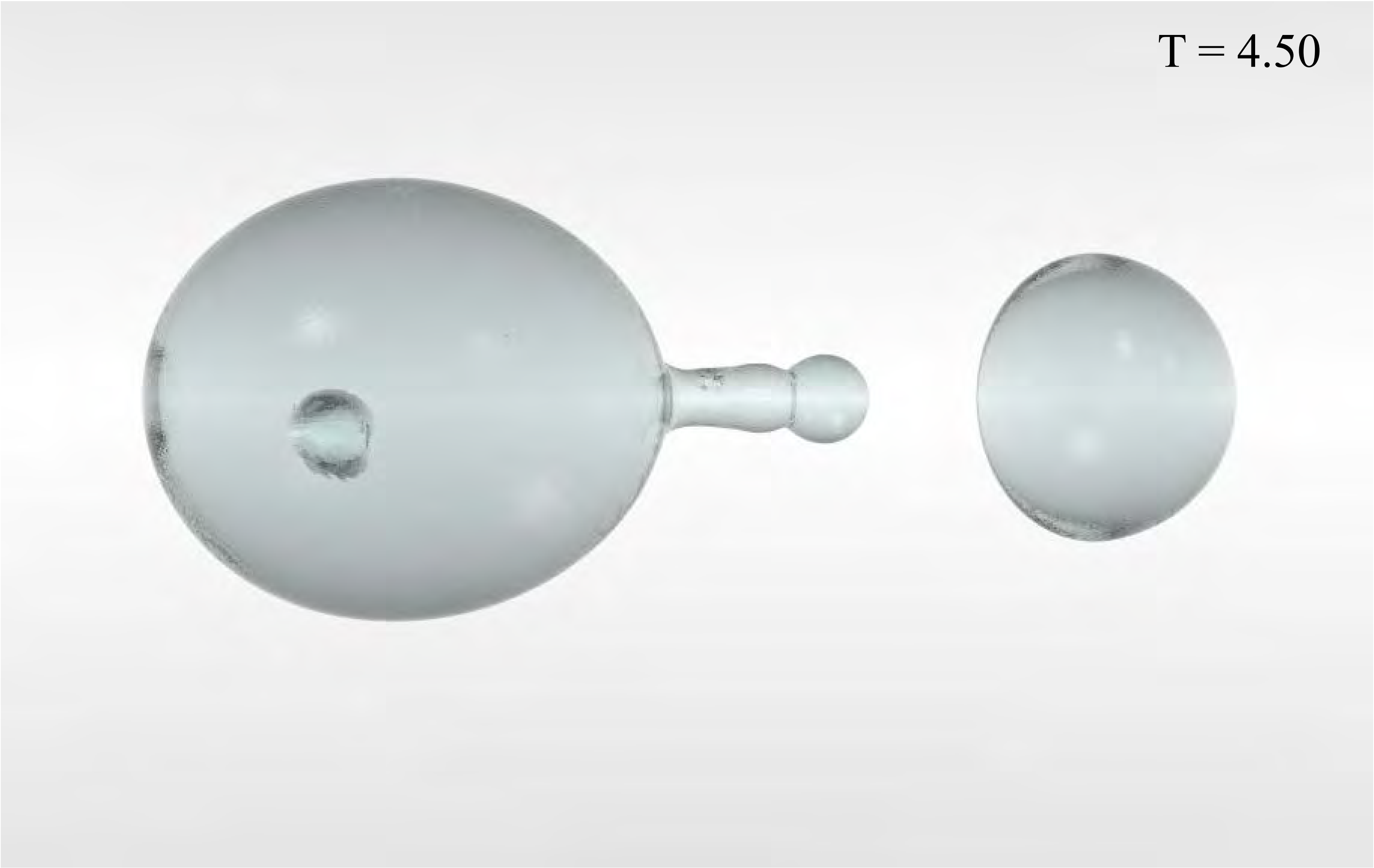
T = 2.00

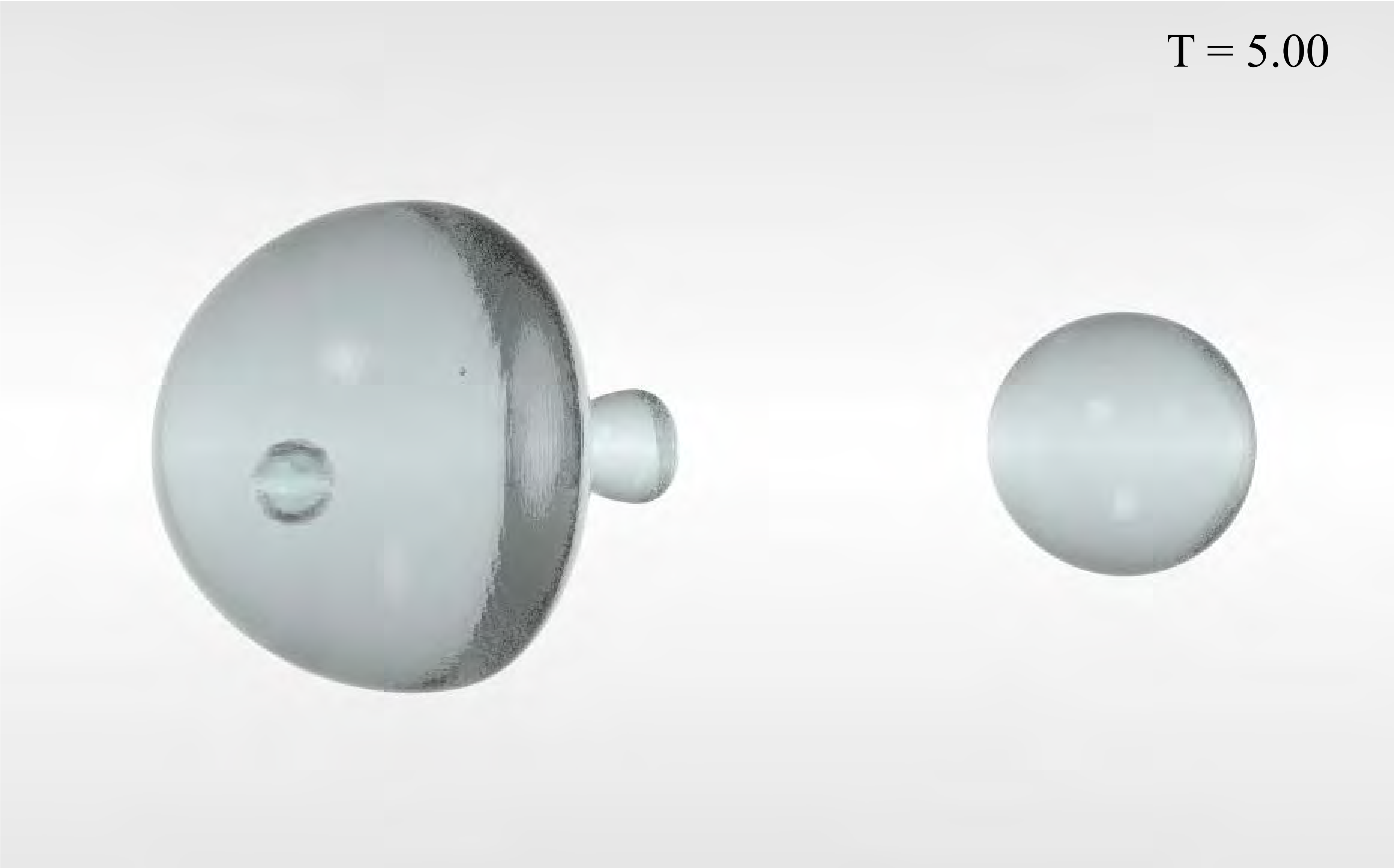

T = 2.50

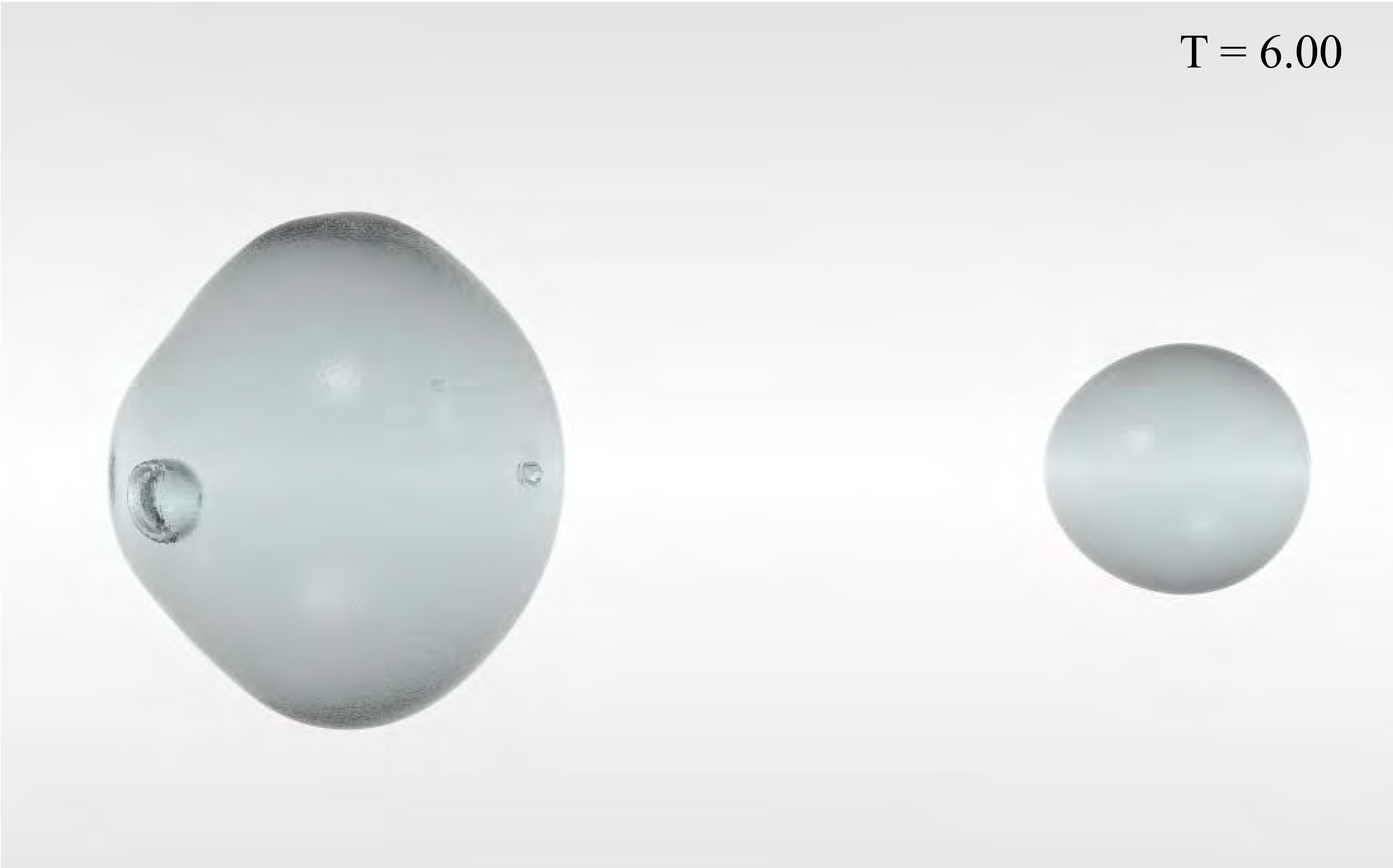

T = 3.00


T = 3.50


T = 4.00


T = 4.50


T = 5.00


T = 6.00

Unequal Coalescence Collision

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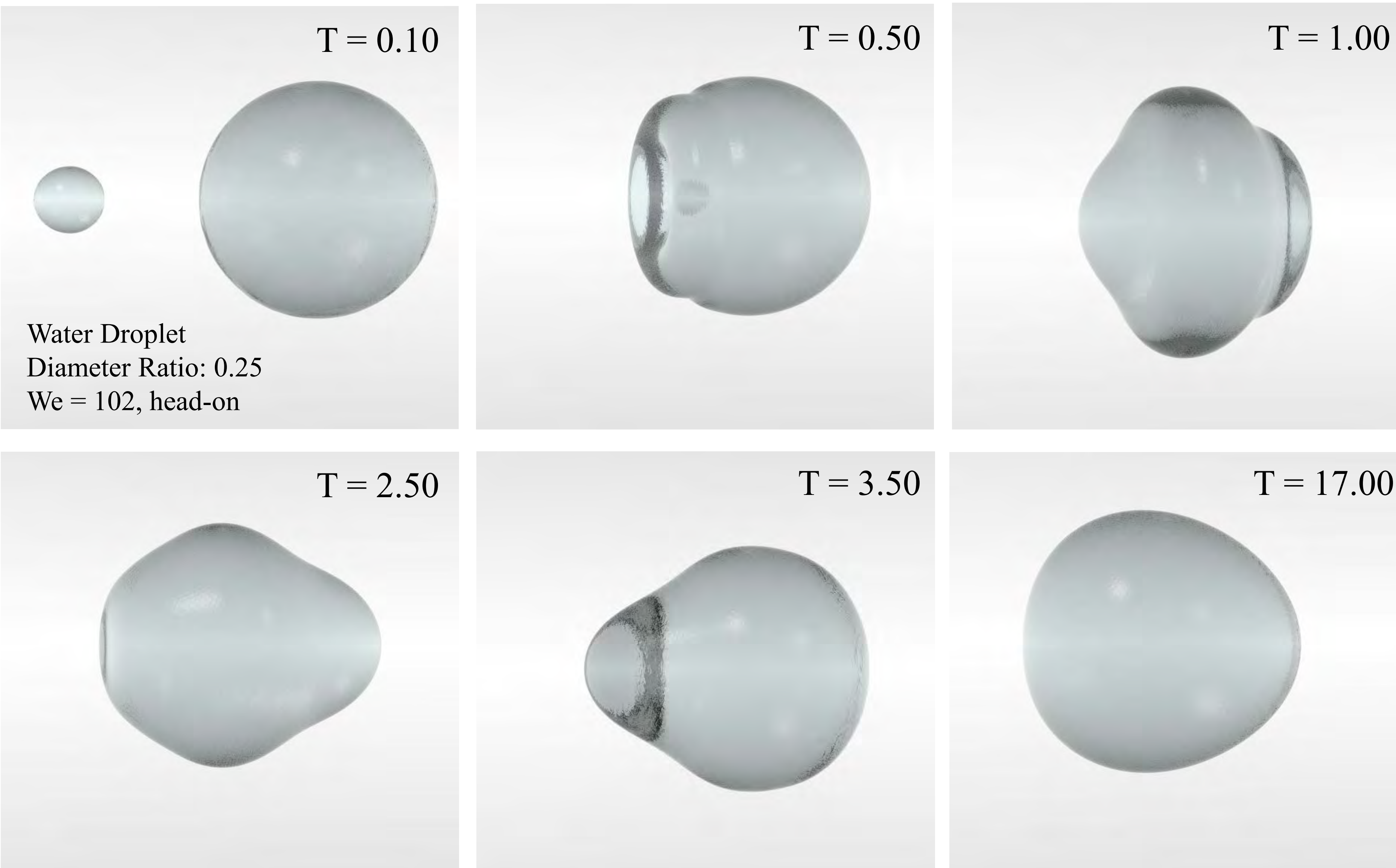
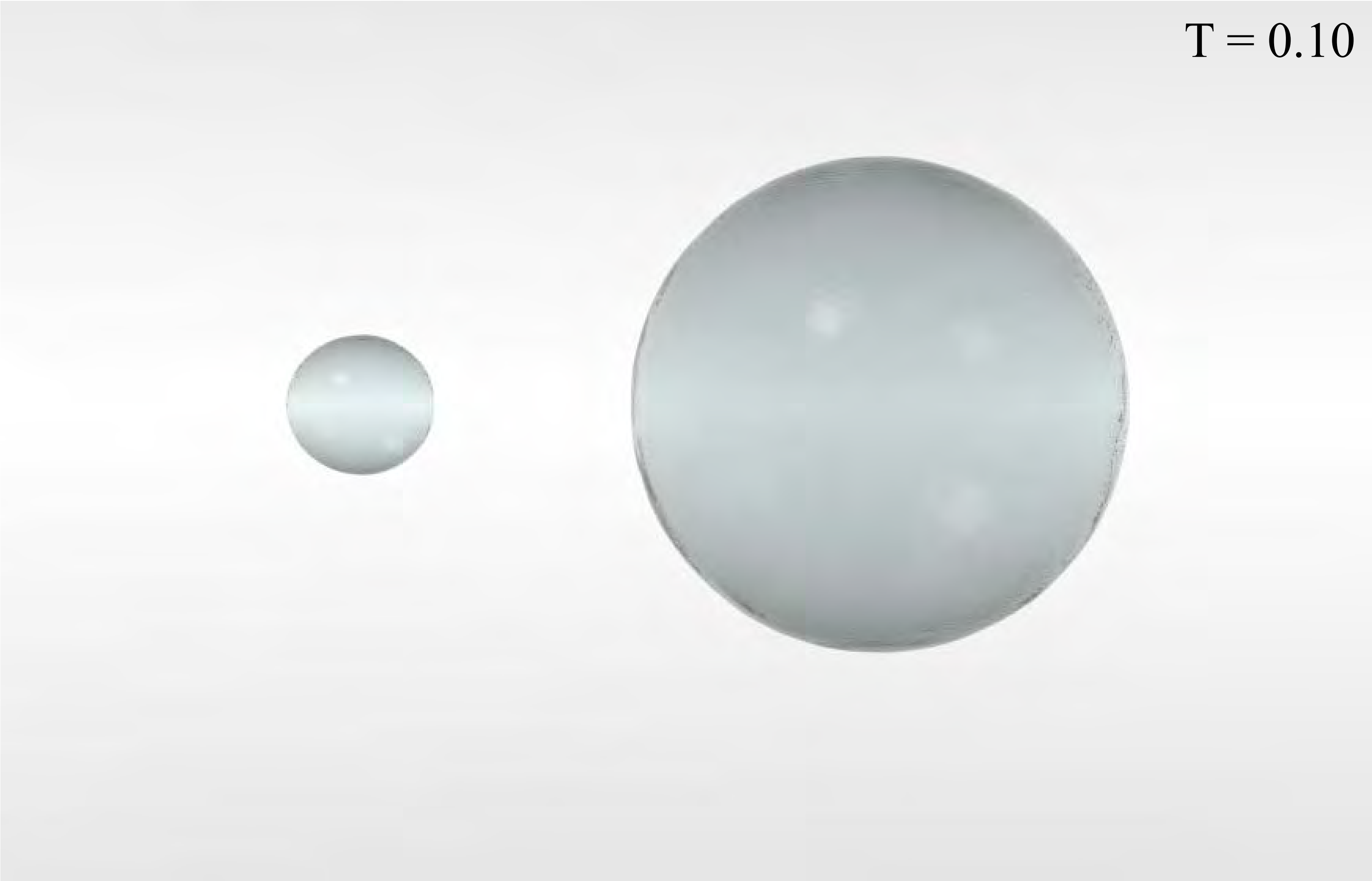
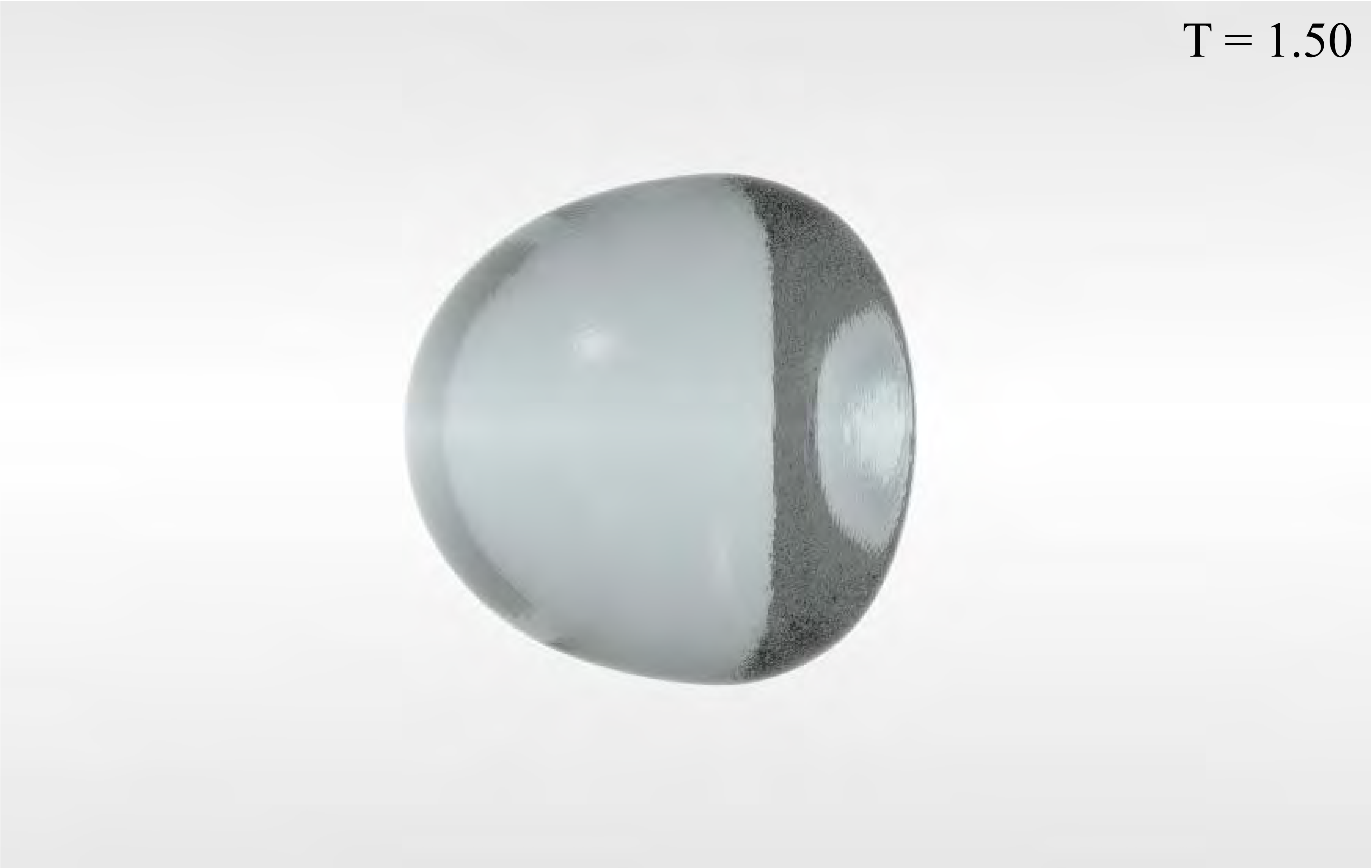



T = 0.10

T = 0.50

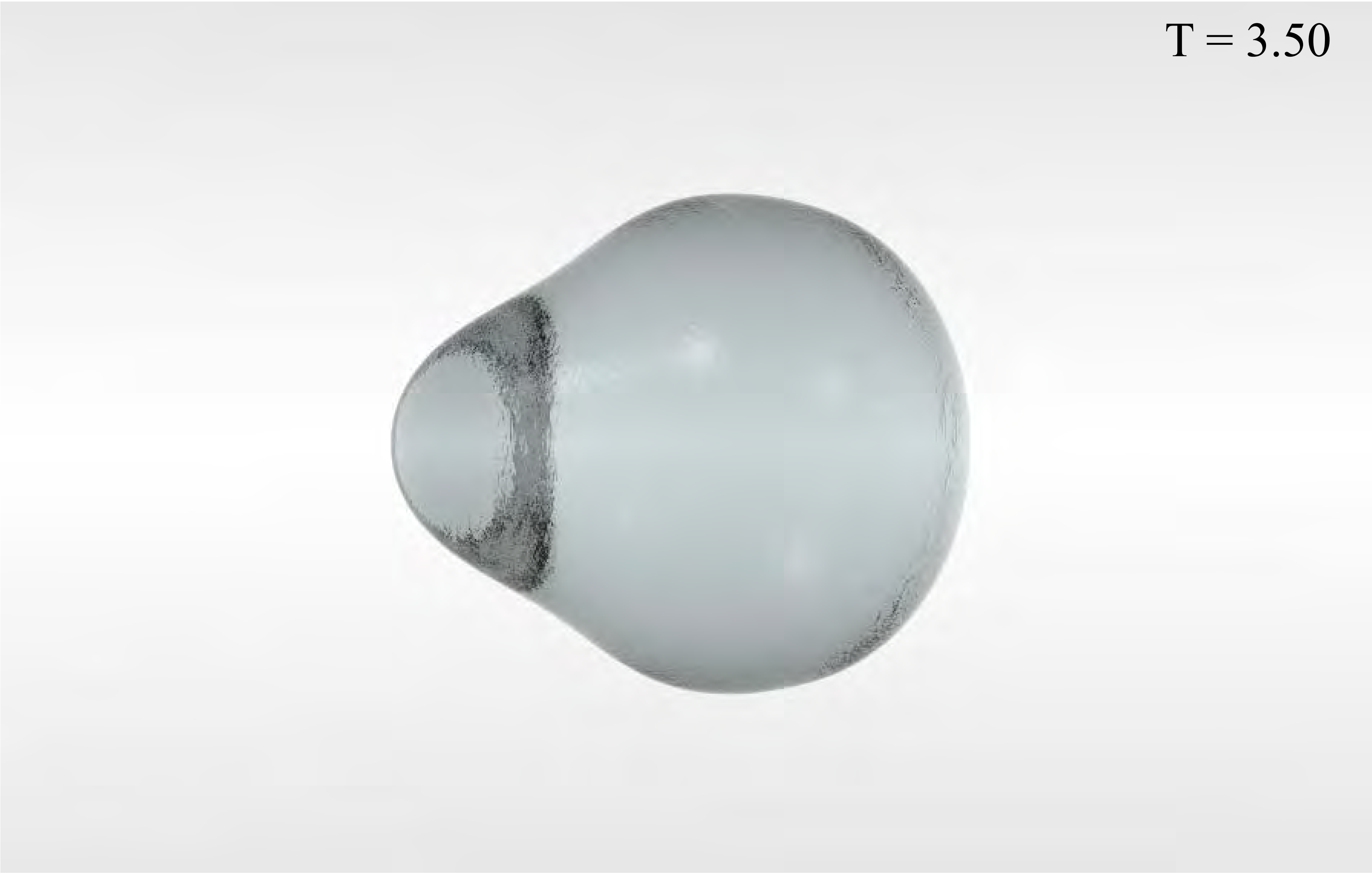

T = 1.00


T = 1.50


T = 2.00


T = 2.50


T = 3.00

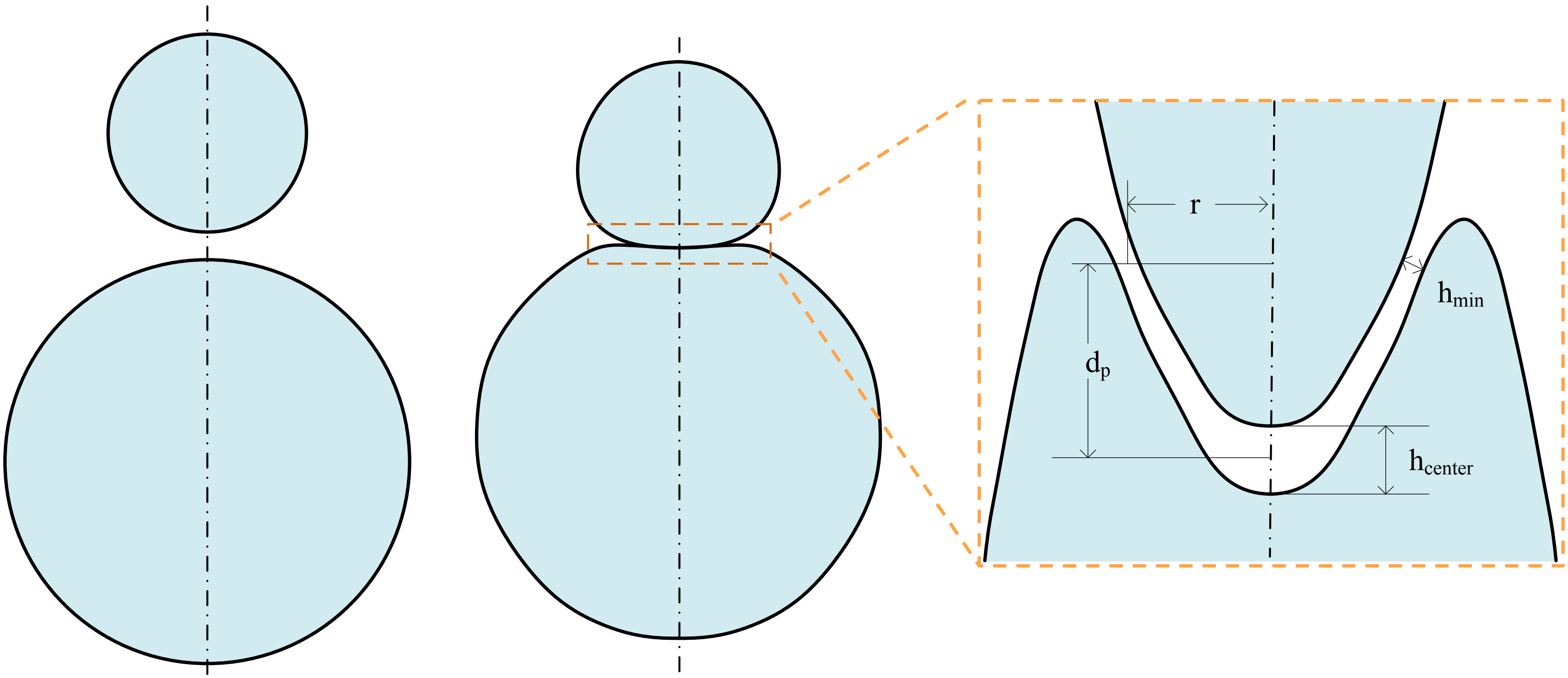

T = 3.50


T = 17.00

Georgia Tech

Thin Gas Film Between Droplets

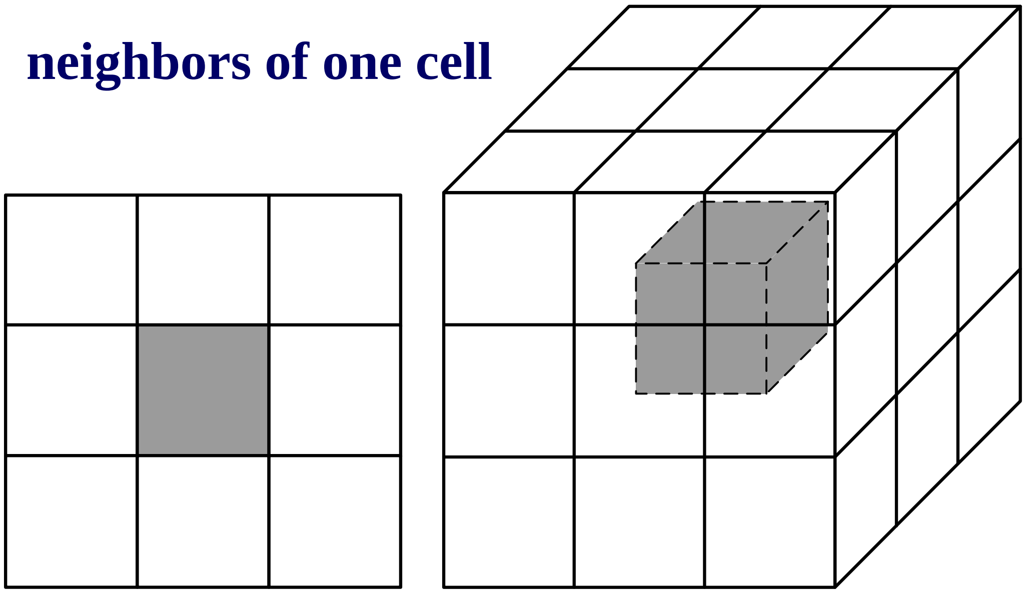
School of Aerospace Engineering

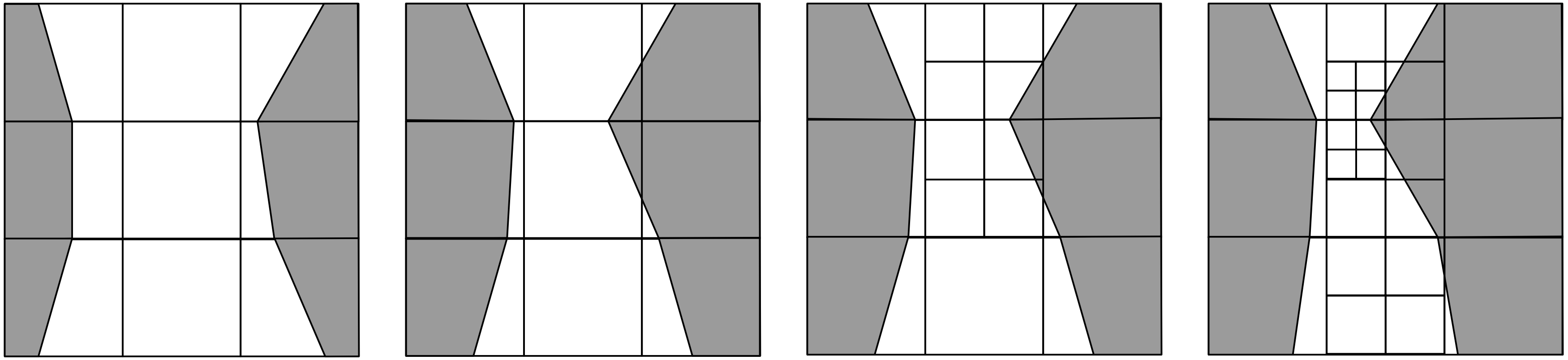


Thickness-based Refinement Criterion Oriented by Digital Topology

neighbors of one cell

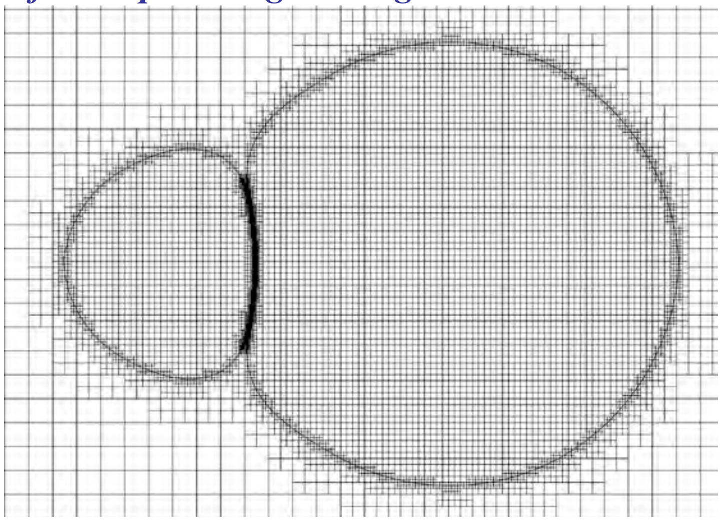
Every interfacial cell must have not less than one neighbor of fully gas phase and not less than one neighbor of fully liquid phase.

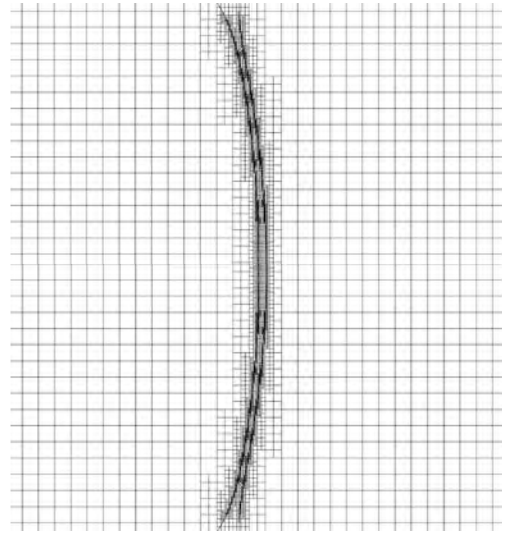




resolved under-resolved refined refined

Thin Gas Film between Two Droplets

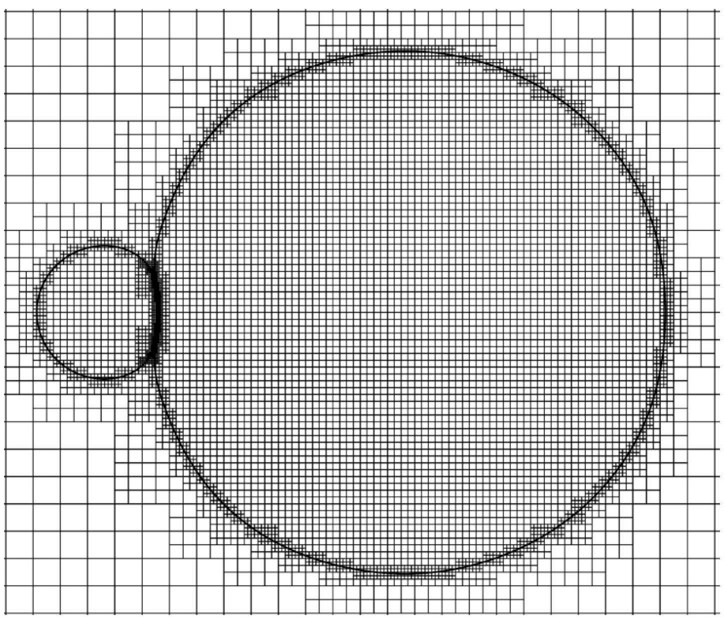


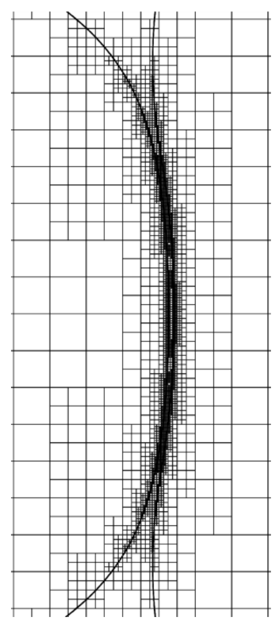


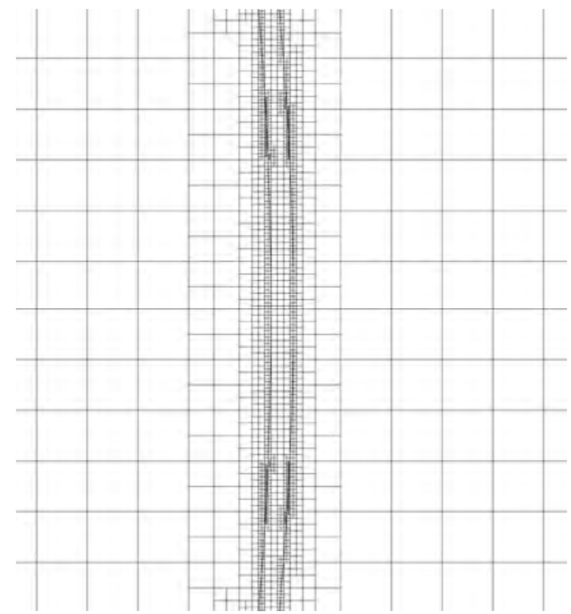
max level : 15

$D_l = 400\ \mu m$

$\Delta x = 0.02\ \mu m$

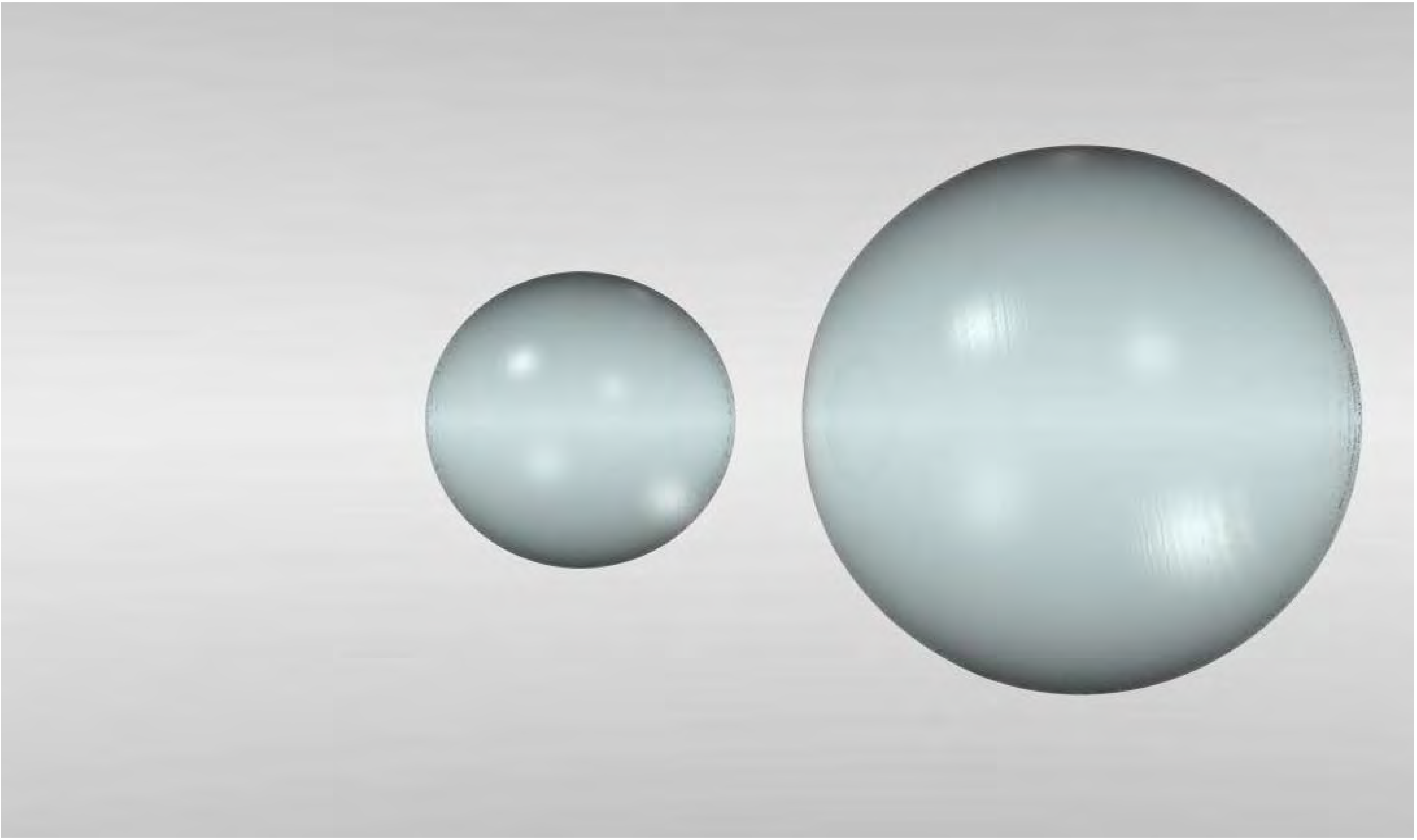






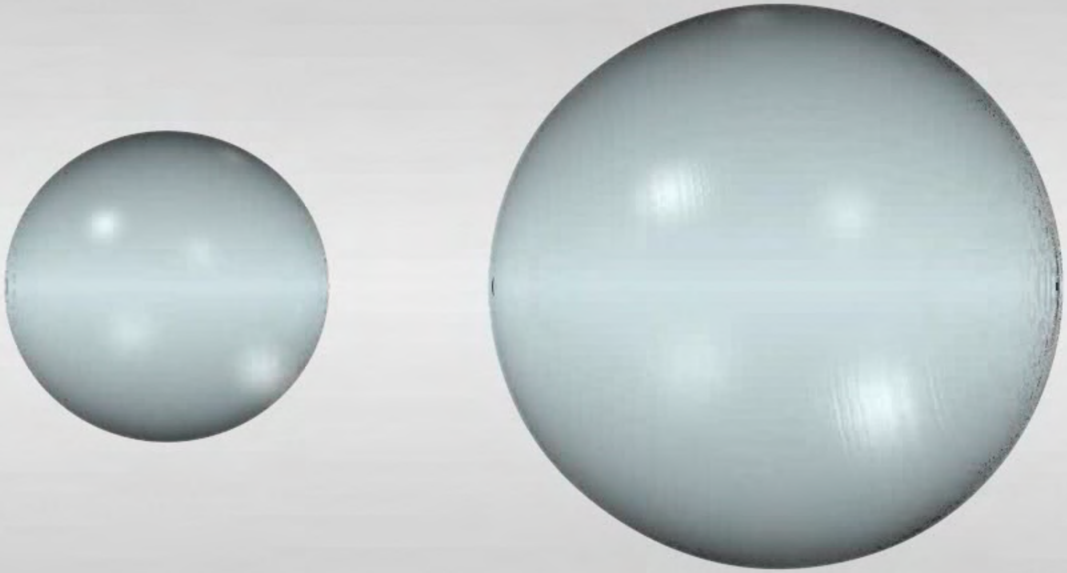
Unequal Bouncing (We = 1)

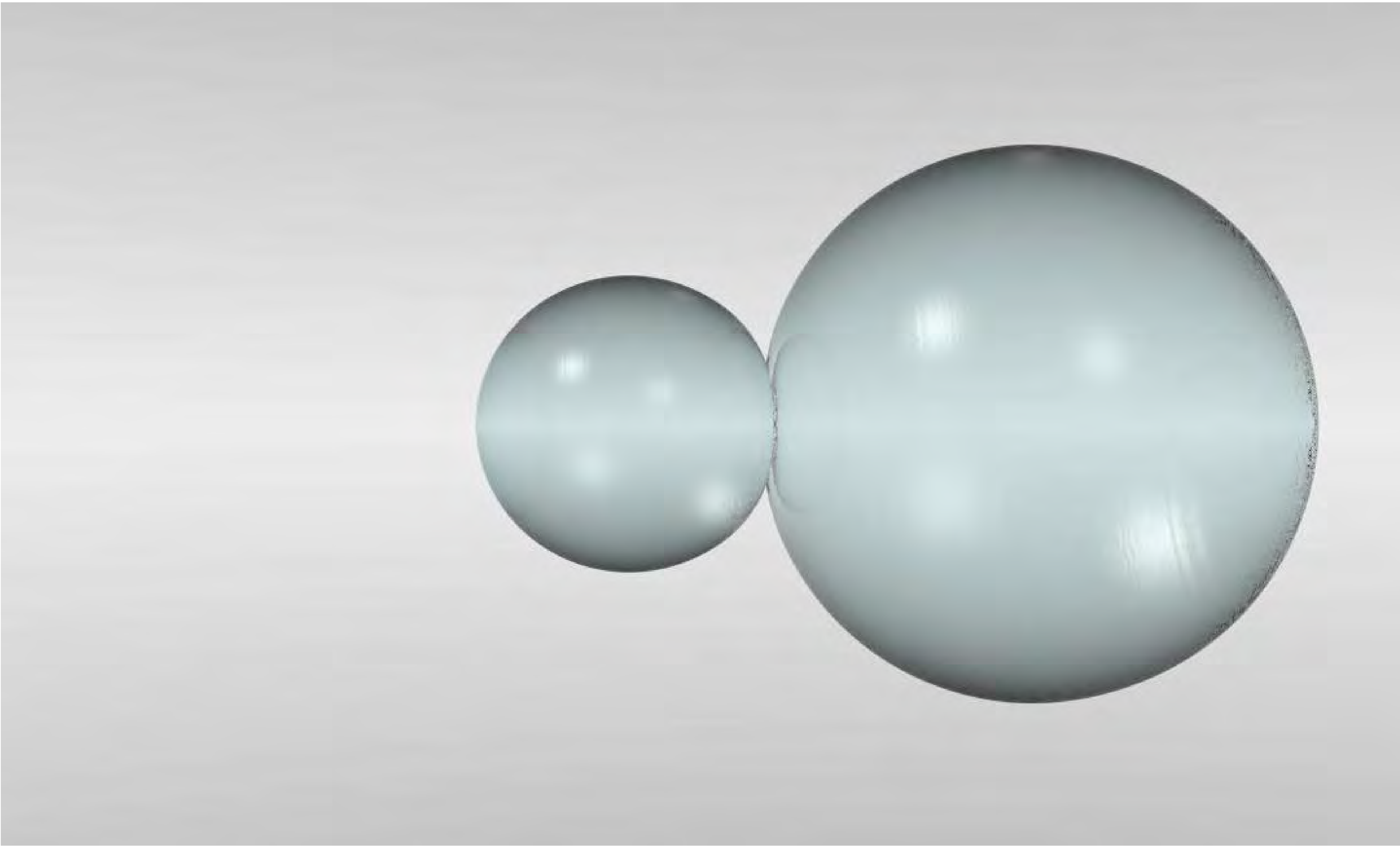
Droplet Diameter Ratio: 0.50

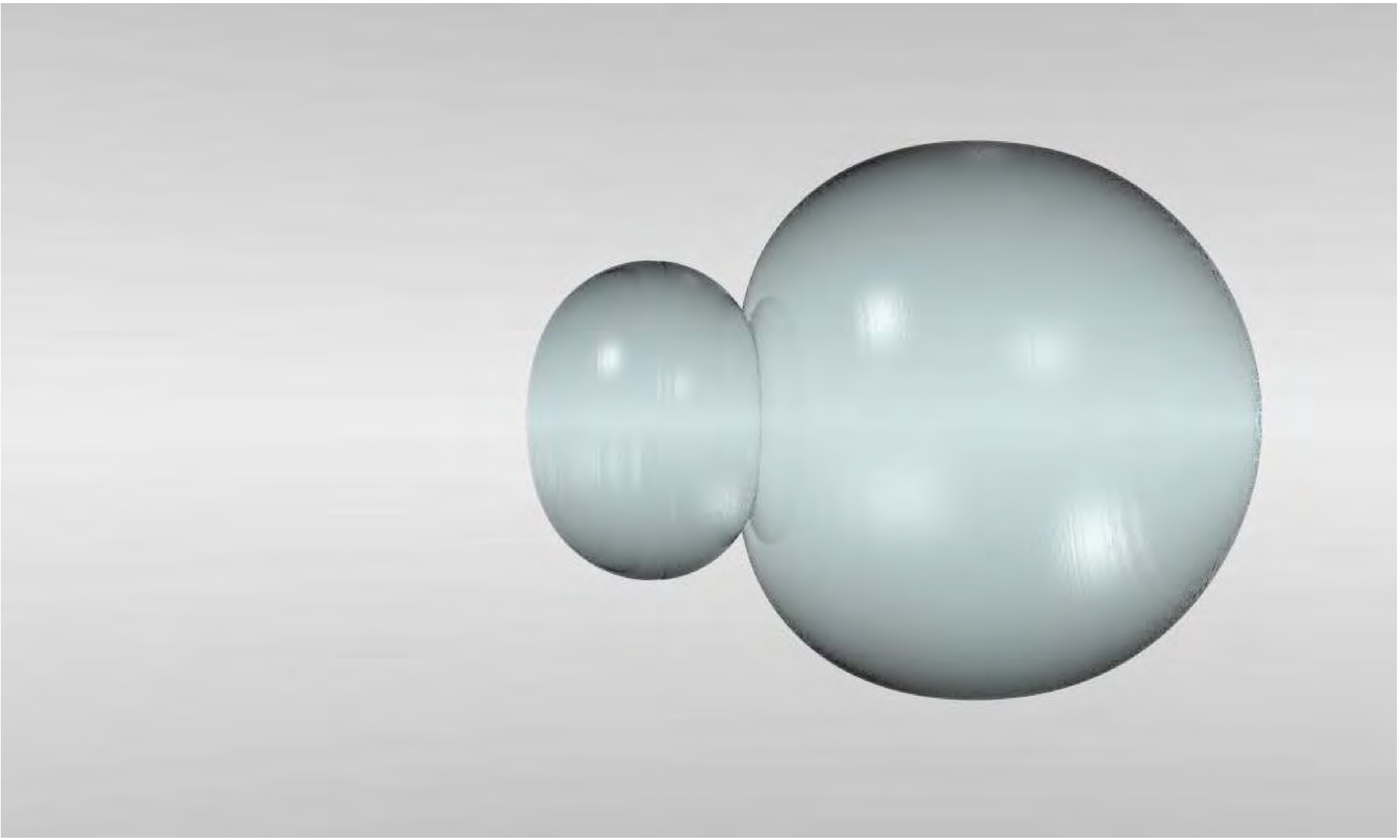


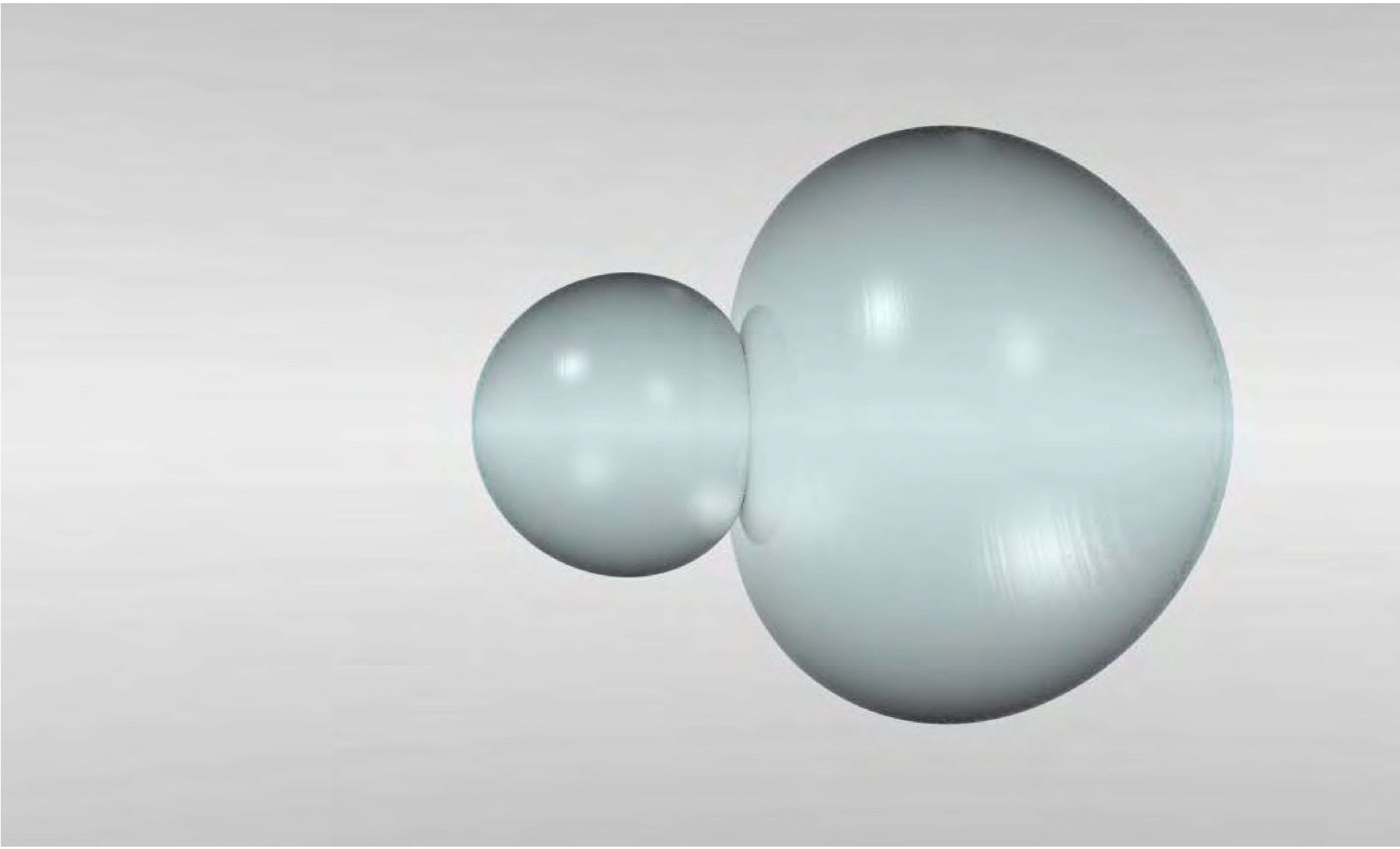
Conditions: water droplets in 1 atm. air, We=1, Re=119.4, B=0, Ds=200 μm, U=0.60 m/s.

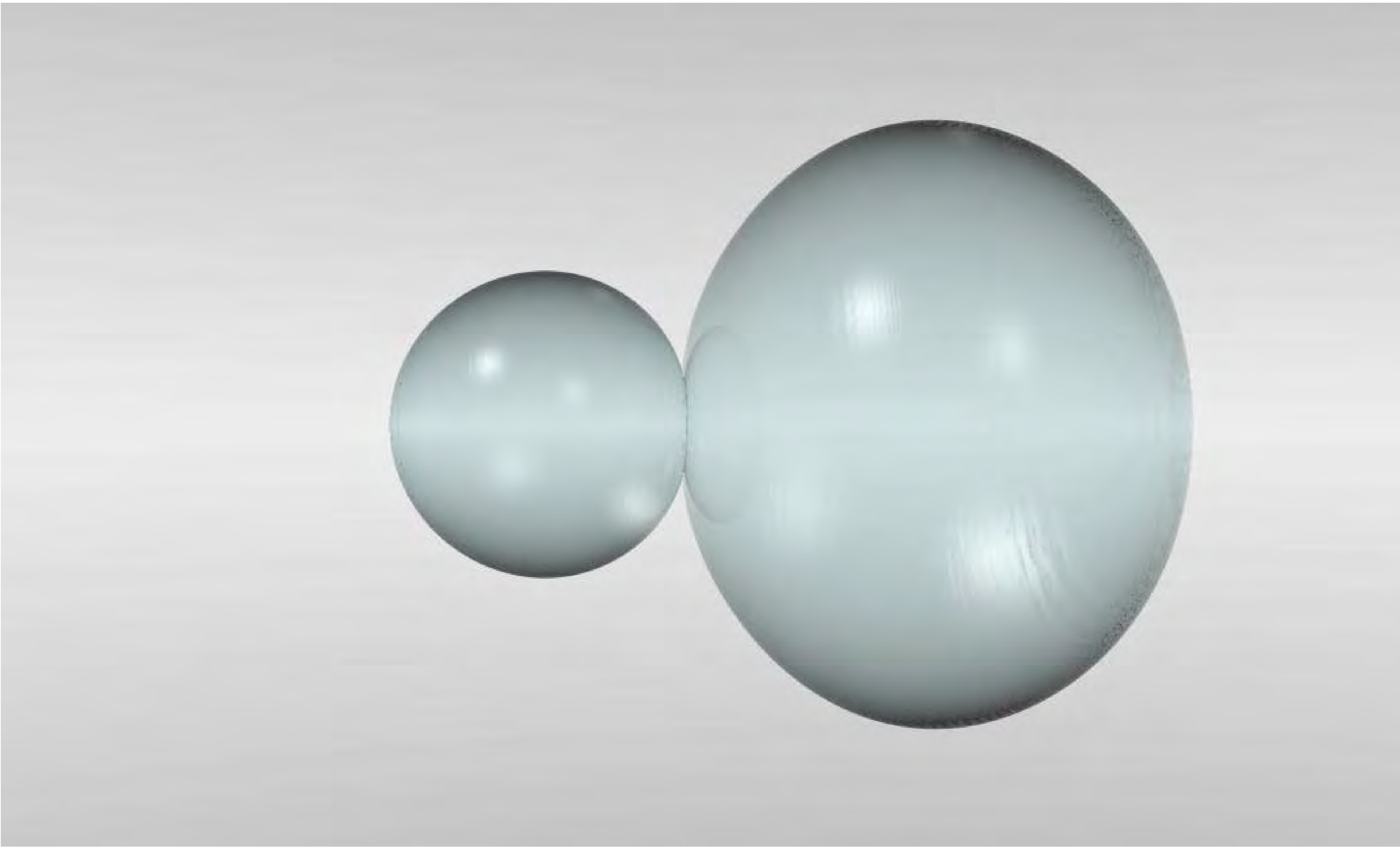
Movie

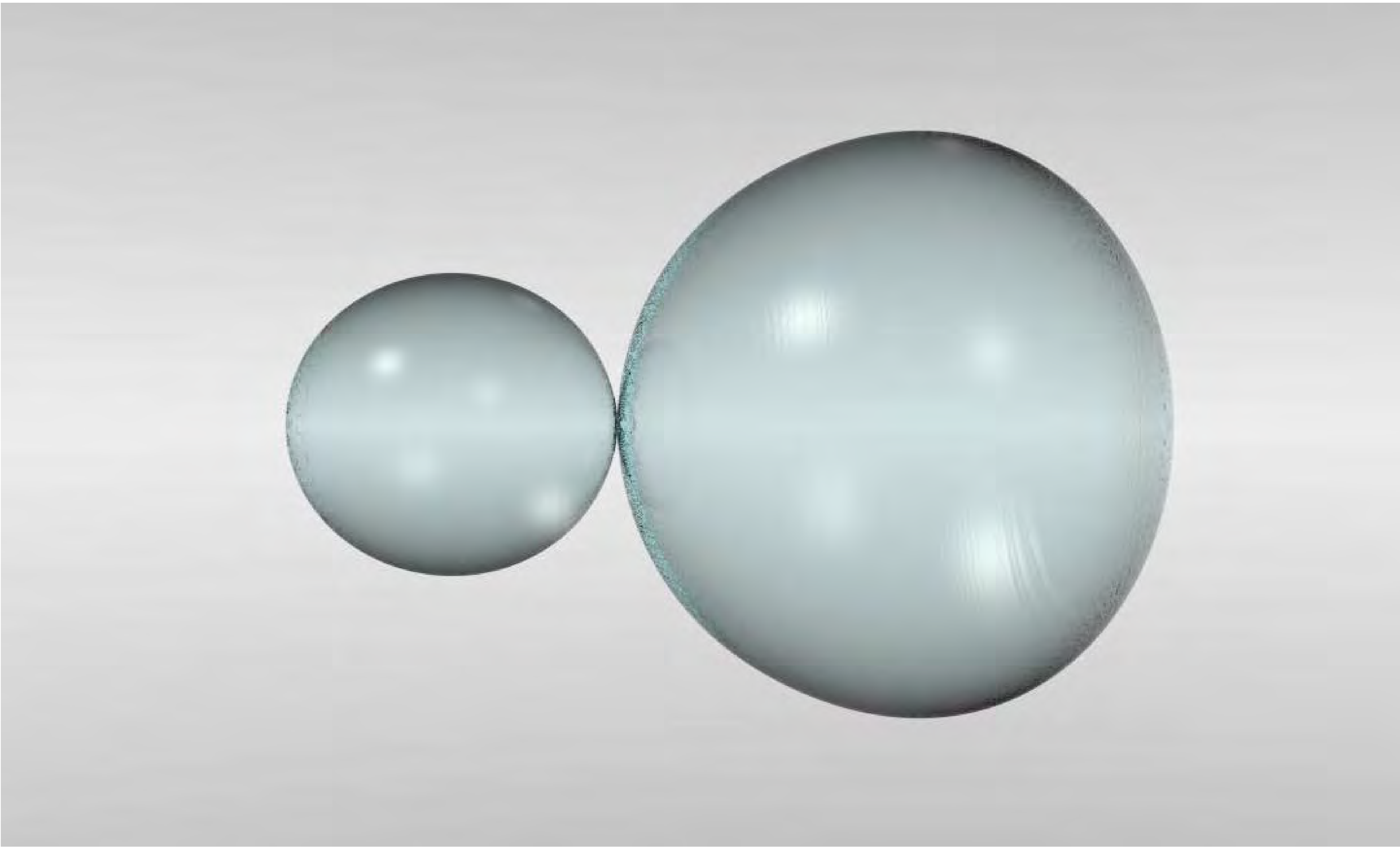


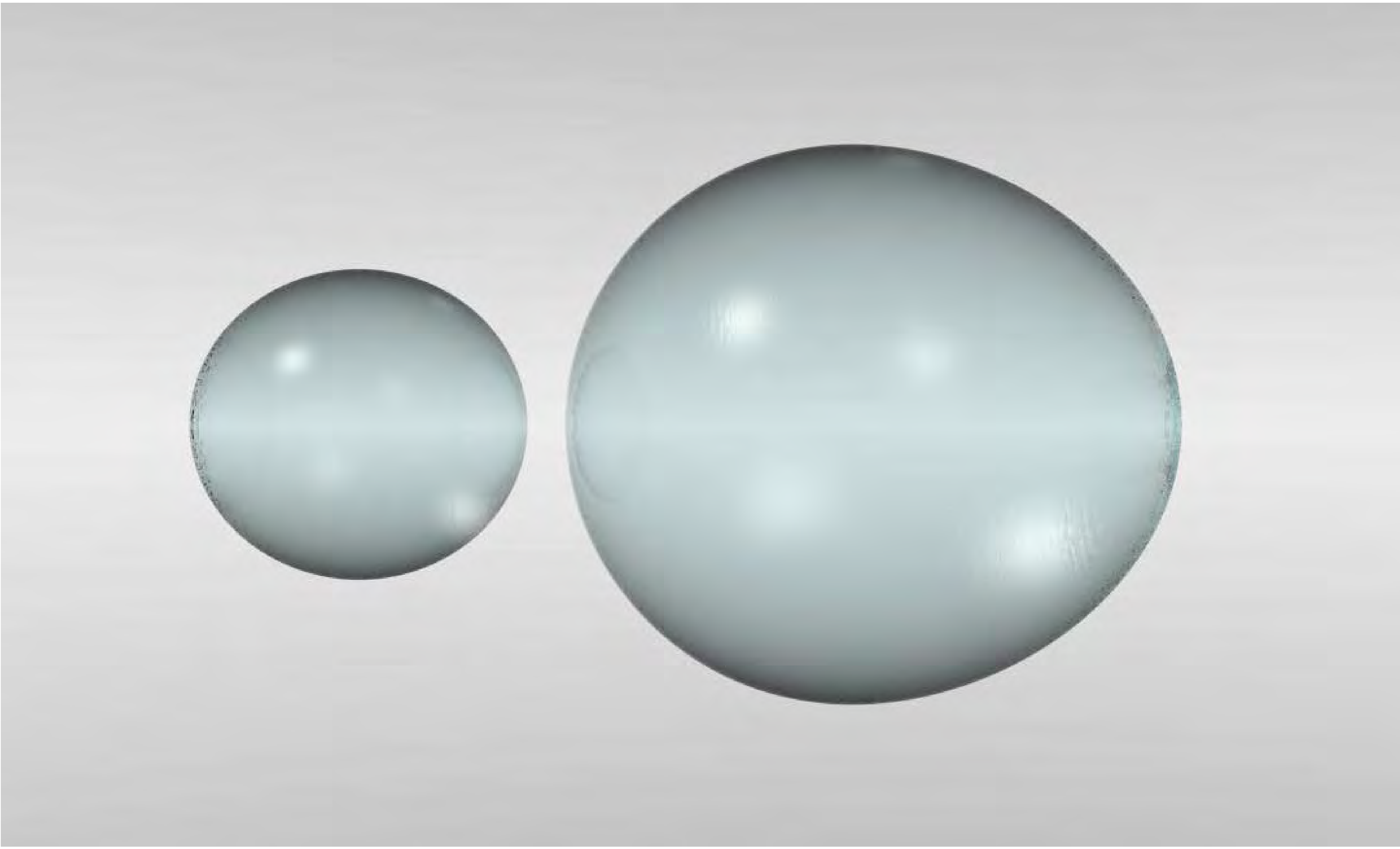


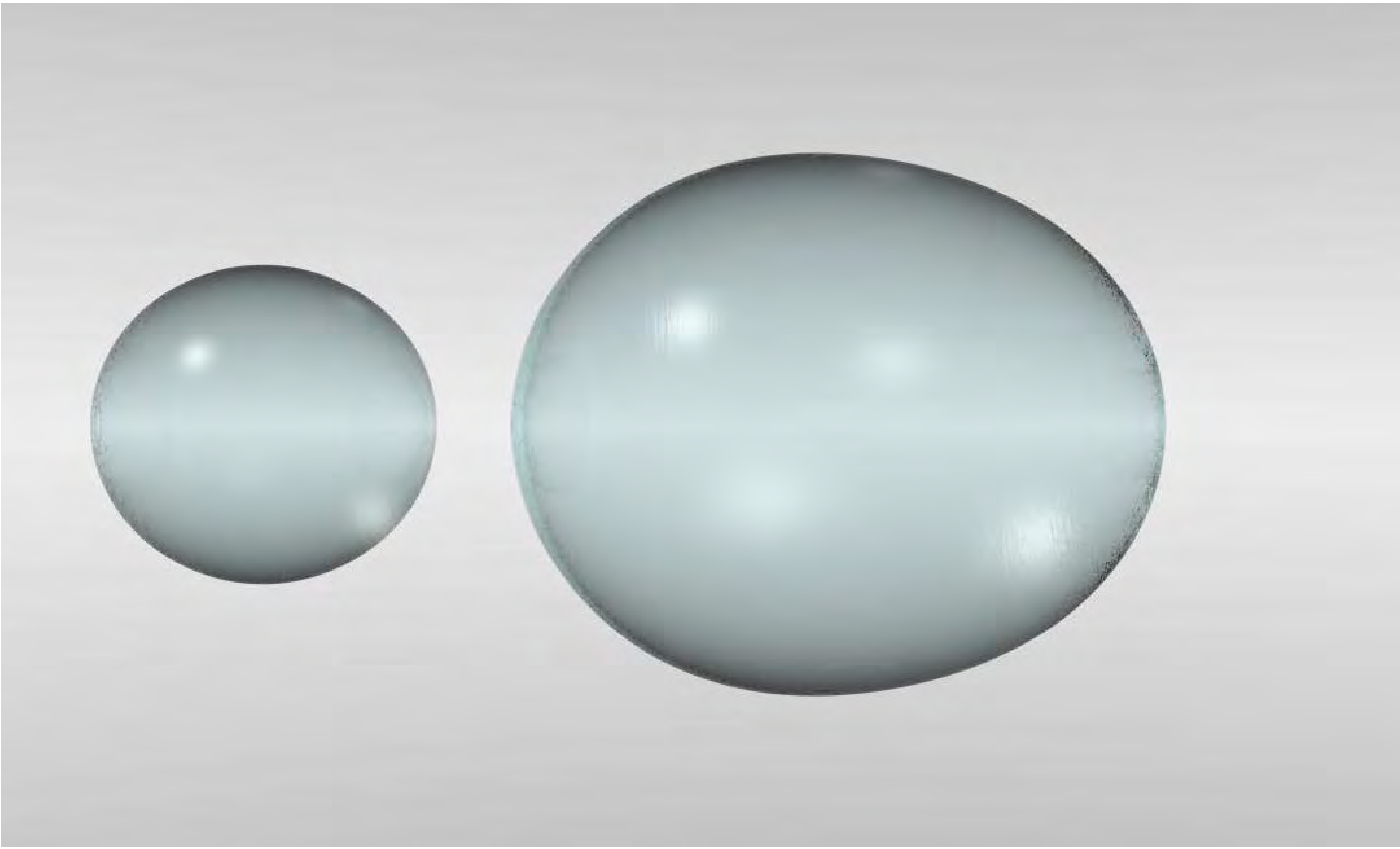






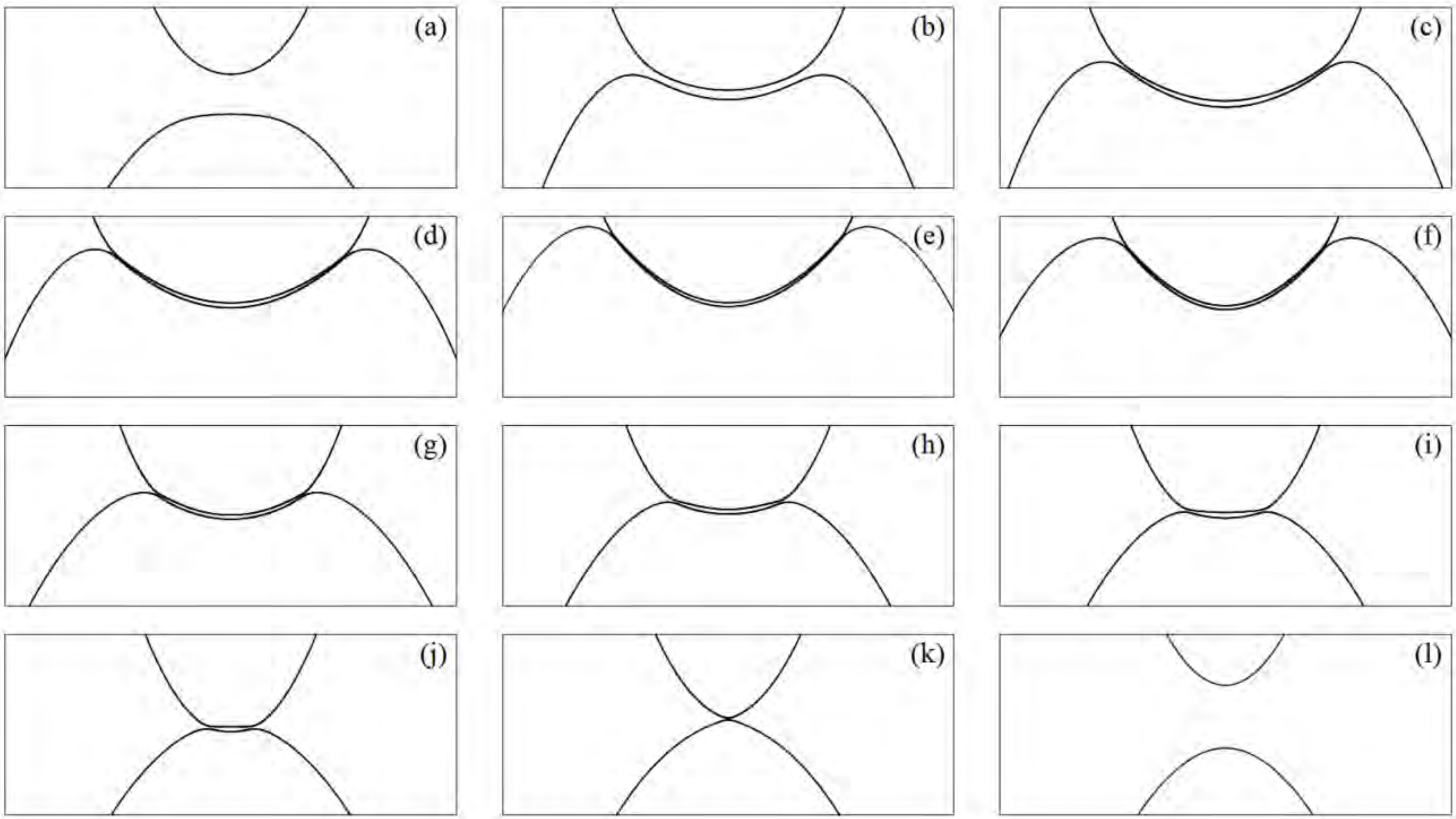






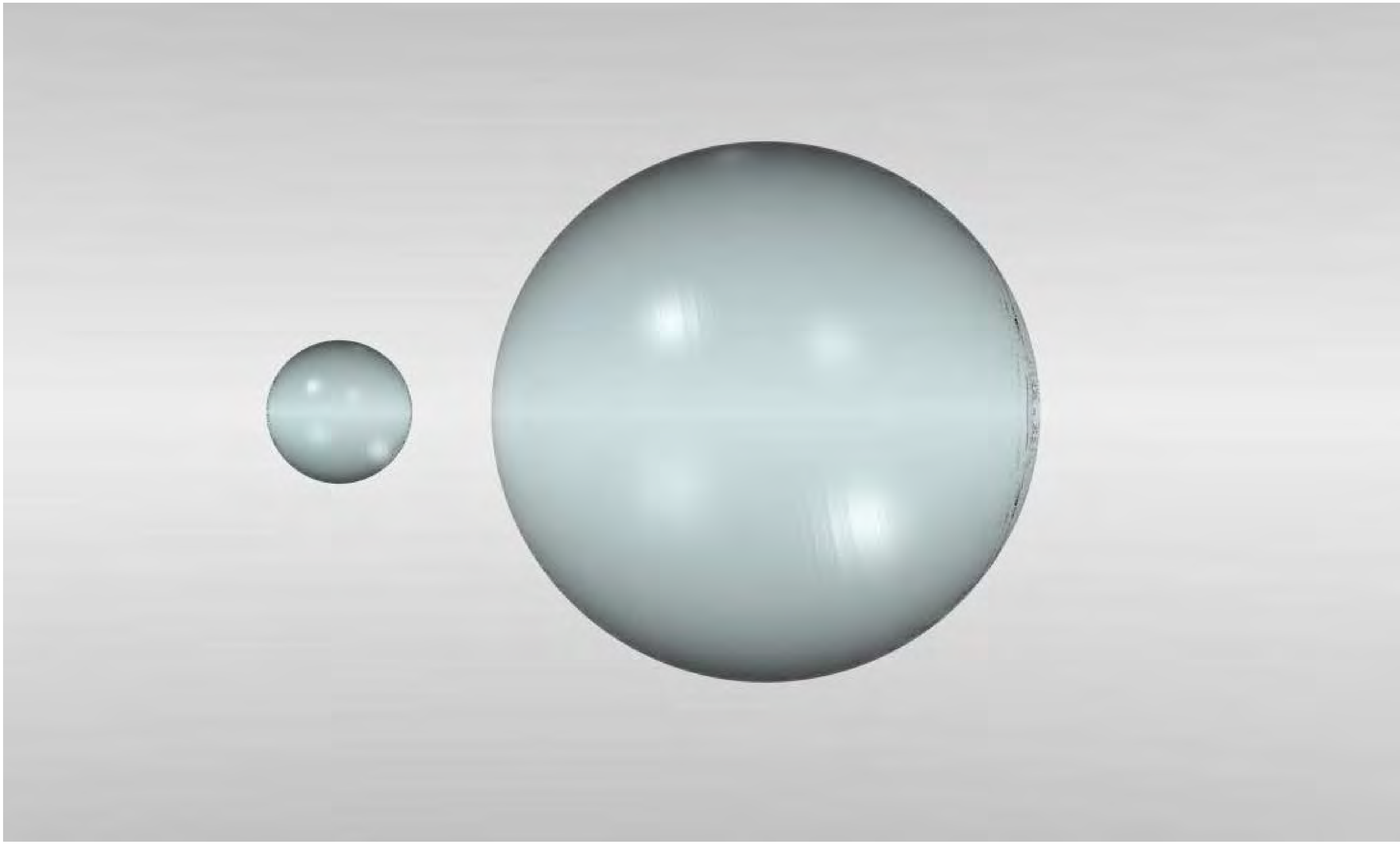
Unequal Bouncing (We = 1)

Droplet Diameter Ratio: 0.50



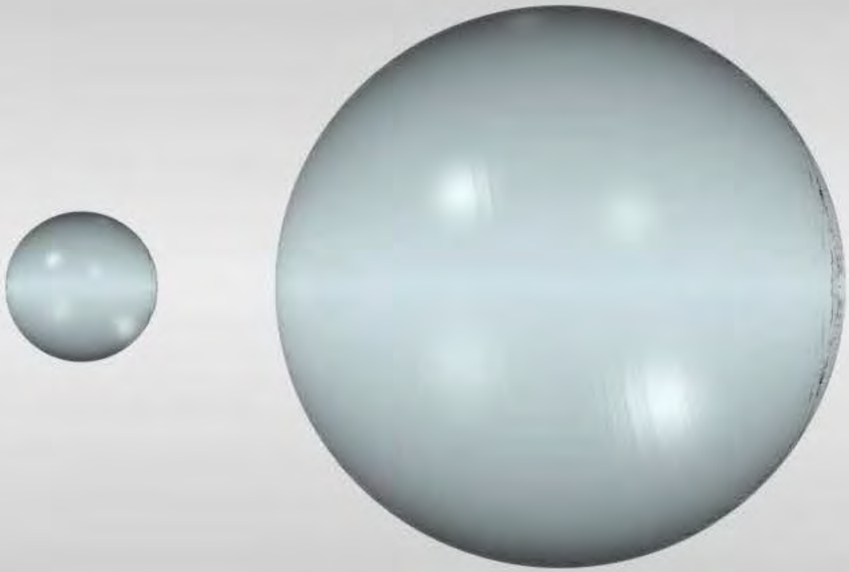
Conditions: water droplets in 1 atm. air, We=1, Re=119.4, B=0, Ds=200 μm, U=0.60 m/s.

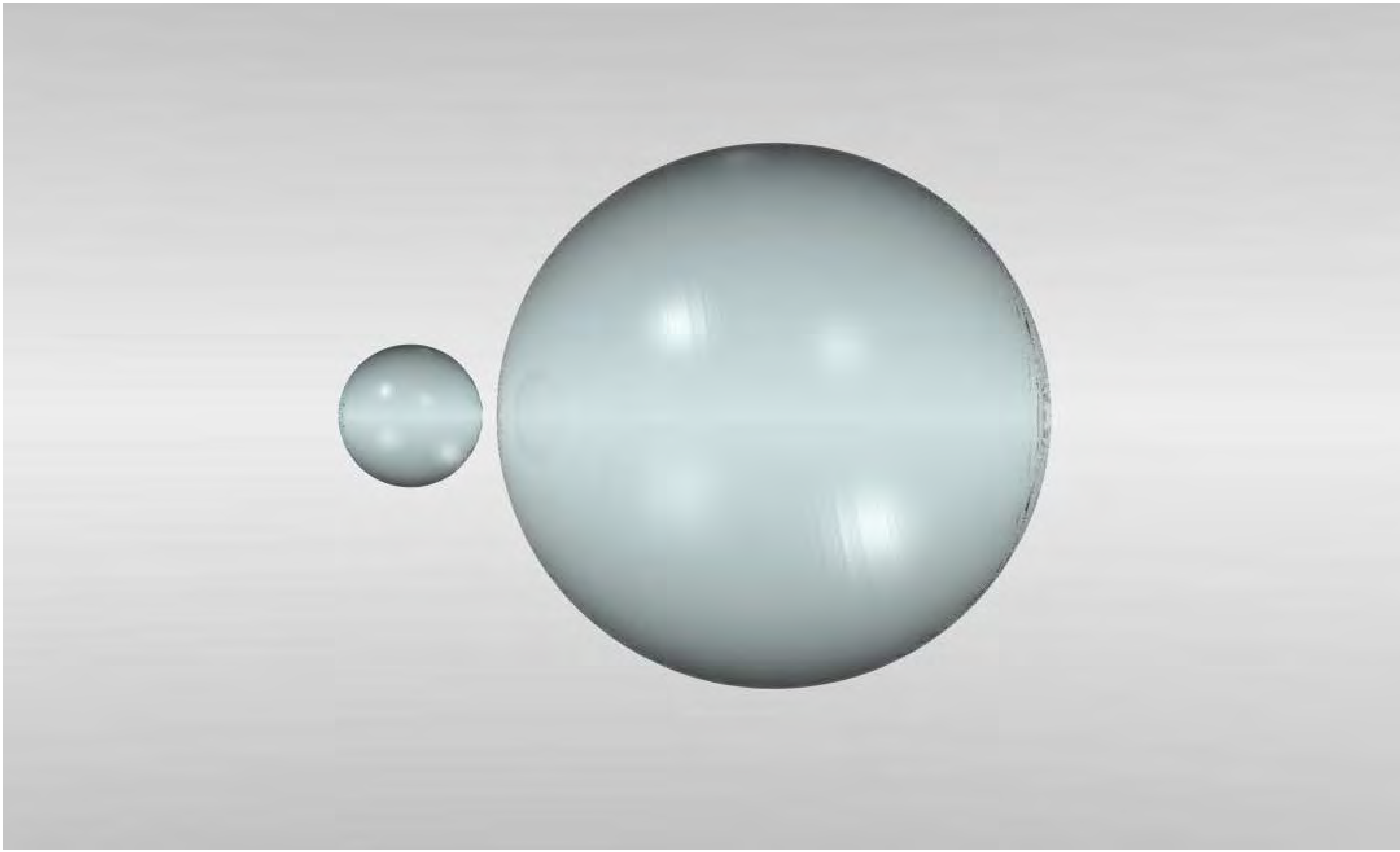
Unequal Bouncing (We = 1)
Droplet Diameter Ratio: 0.25

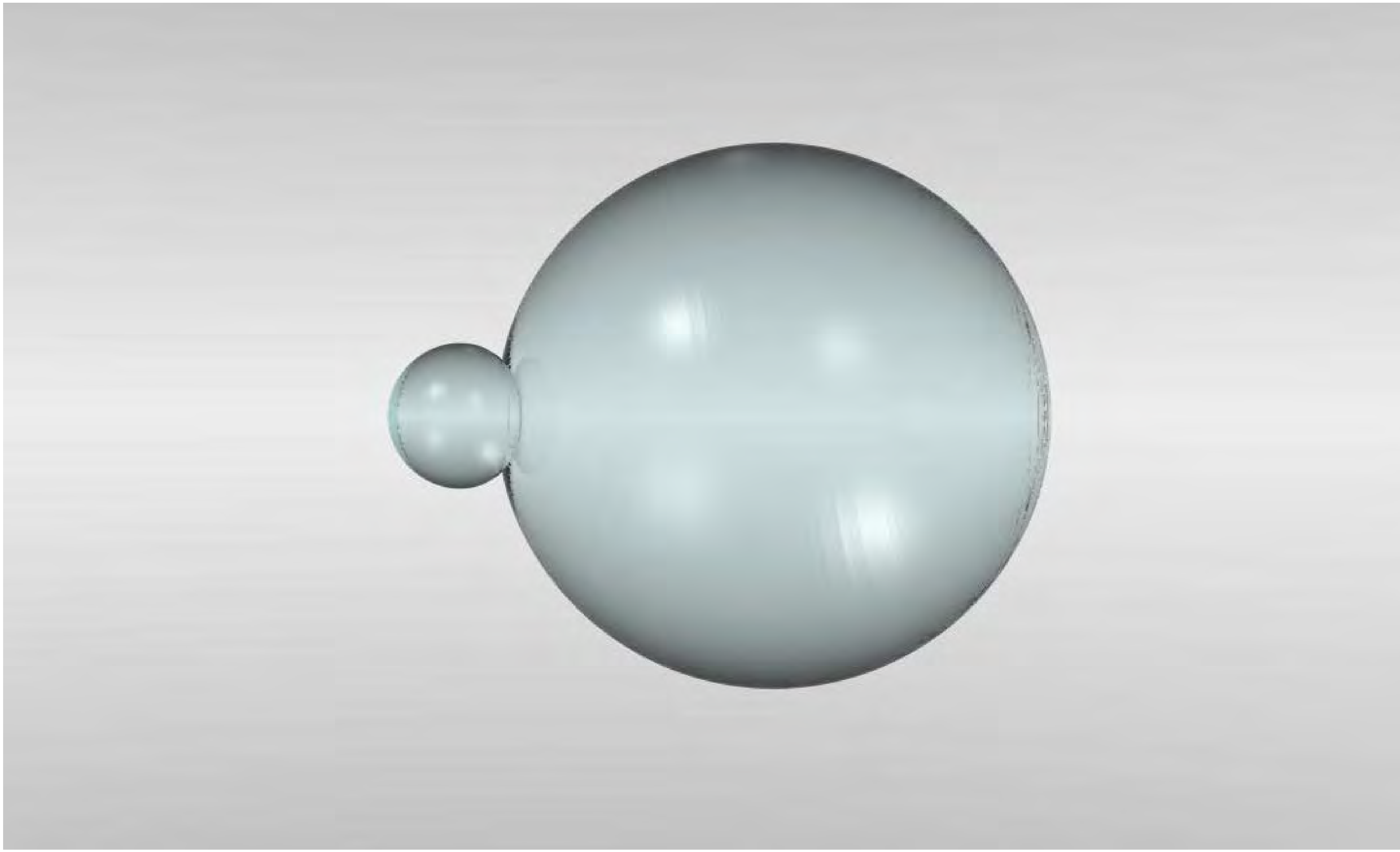


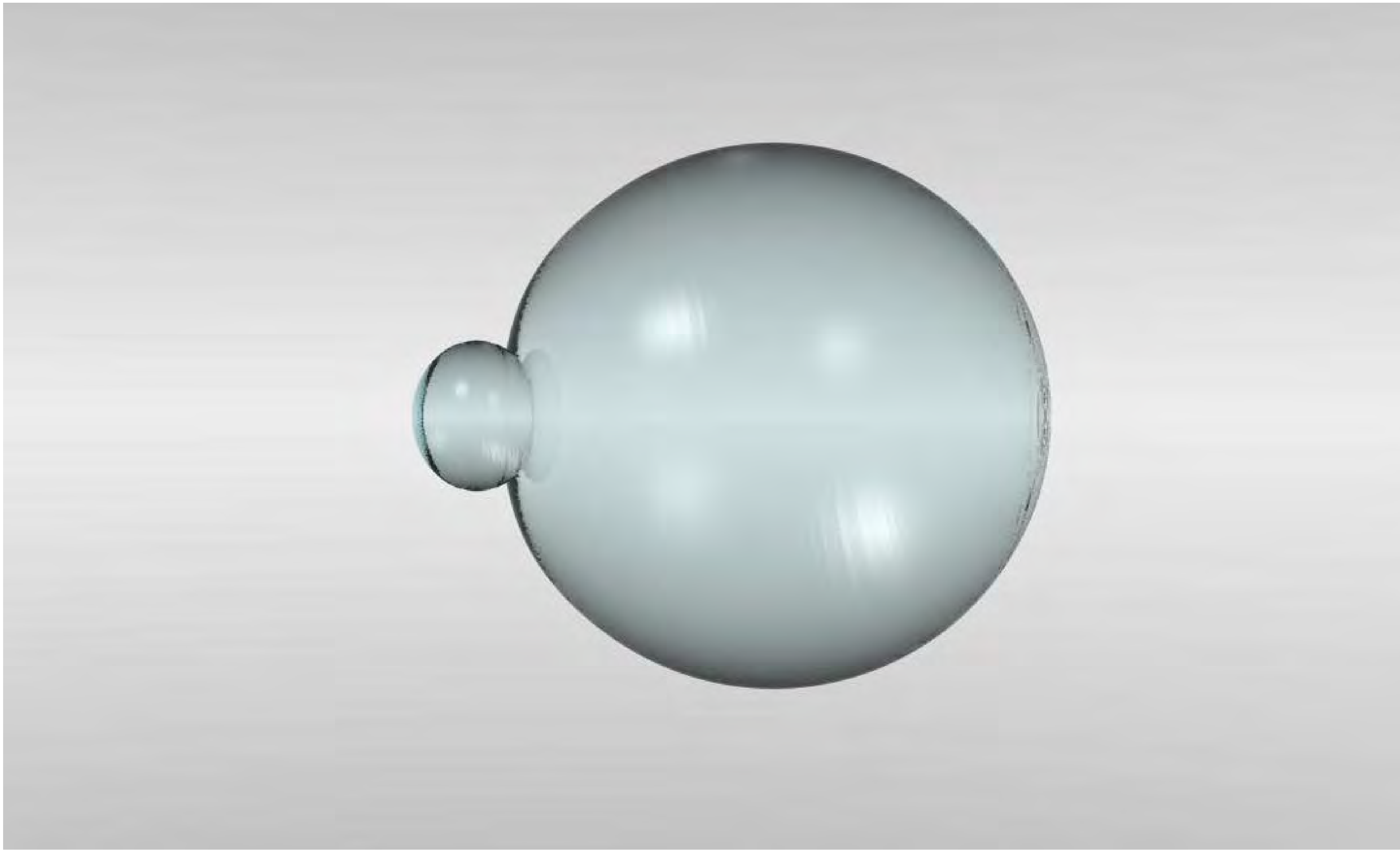
Conditions: water droplets in 1 atm. air, We=1, Re=85.2, B=0, Ds=100 μm, U=0.85 m/s.

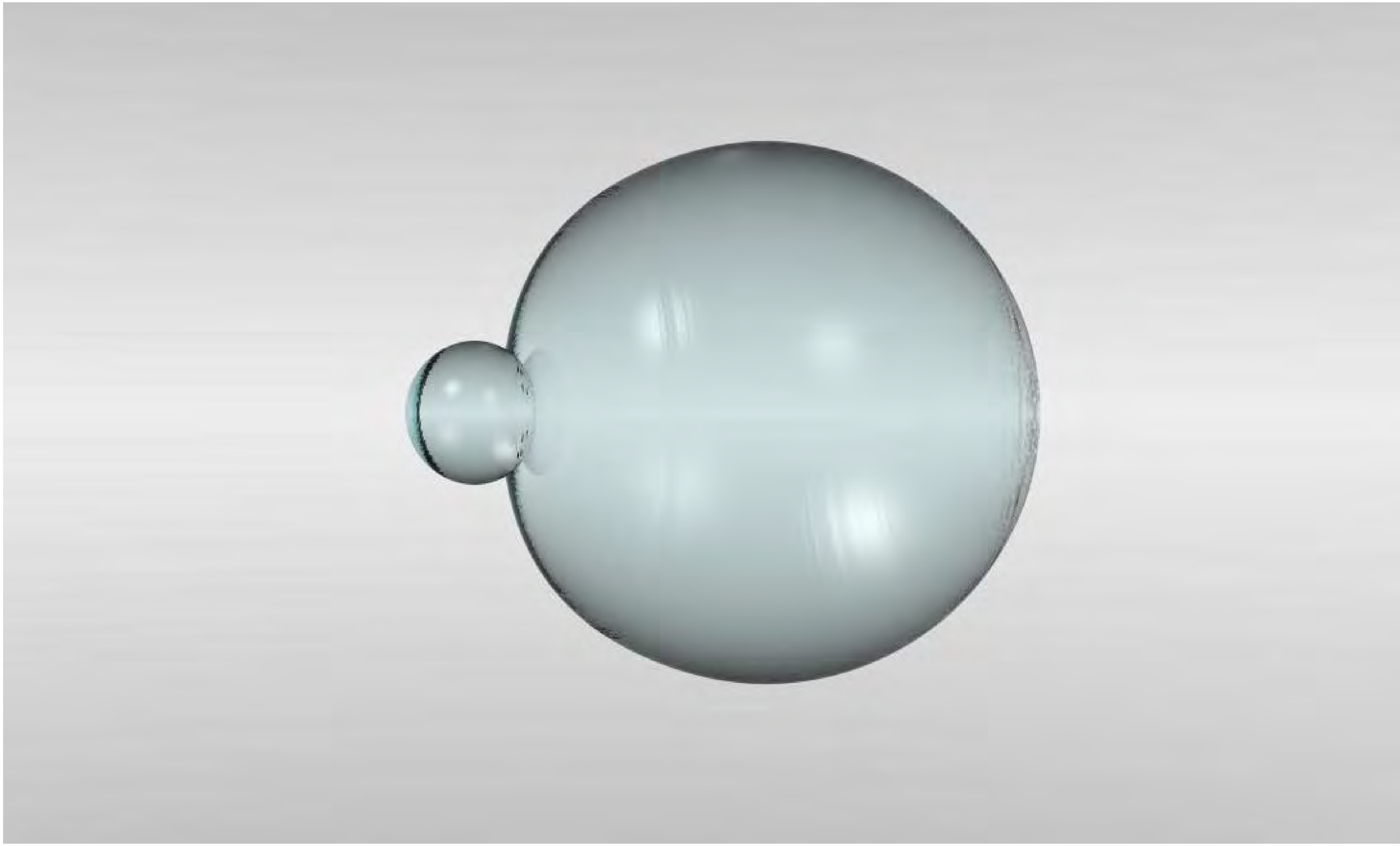
Movie

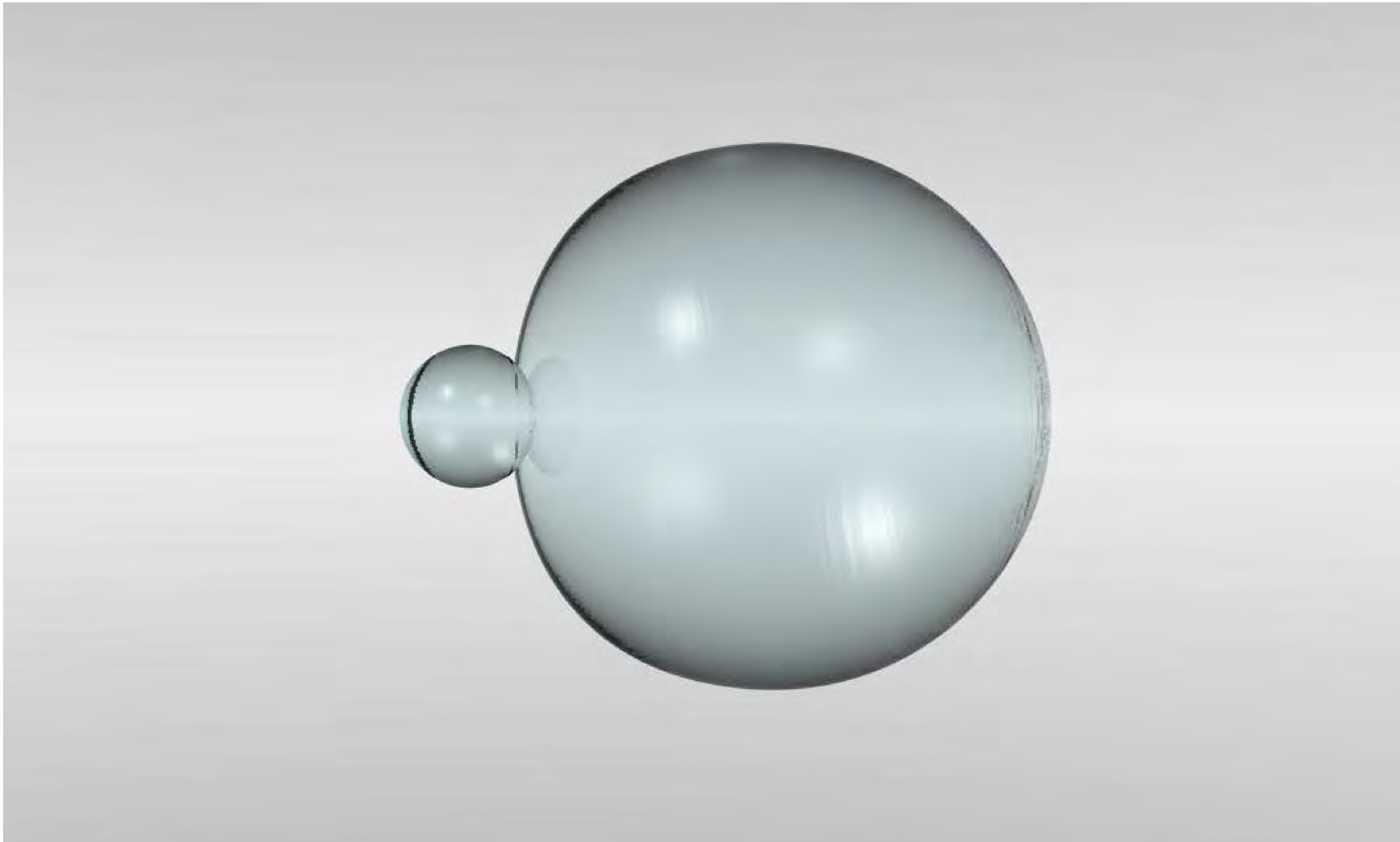


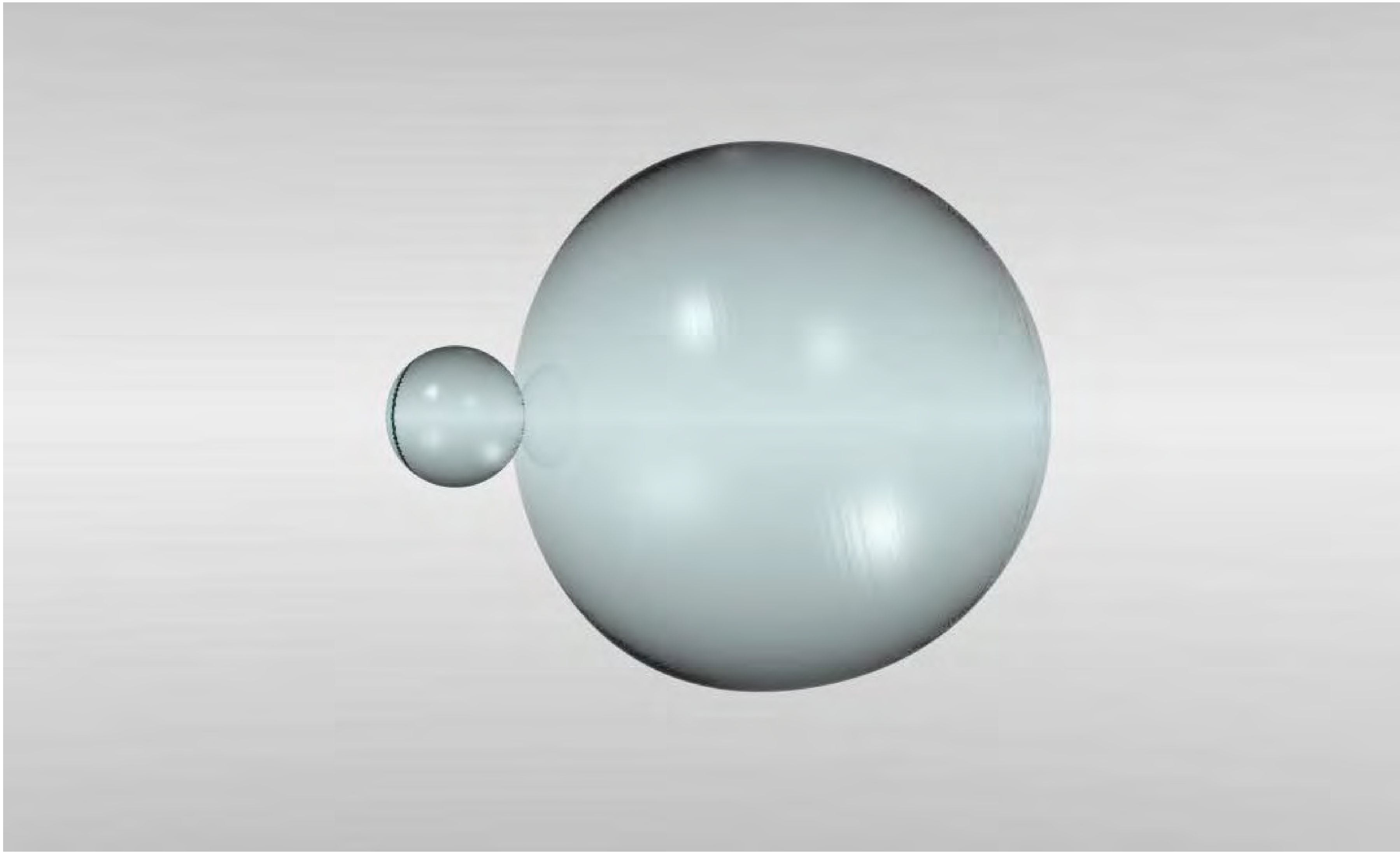


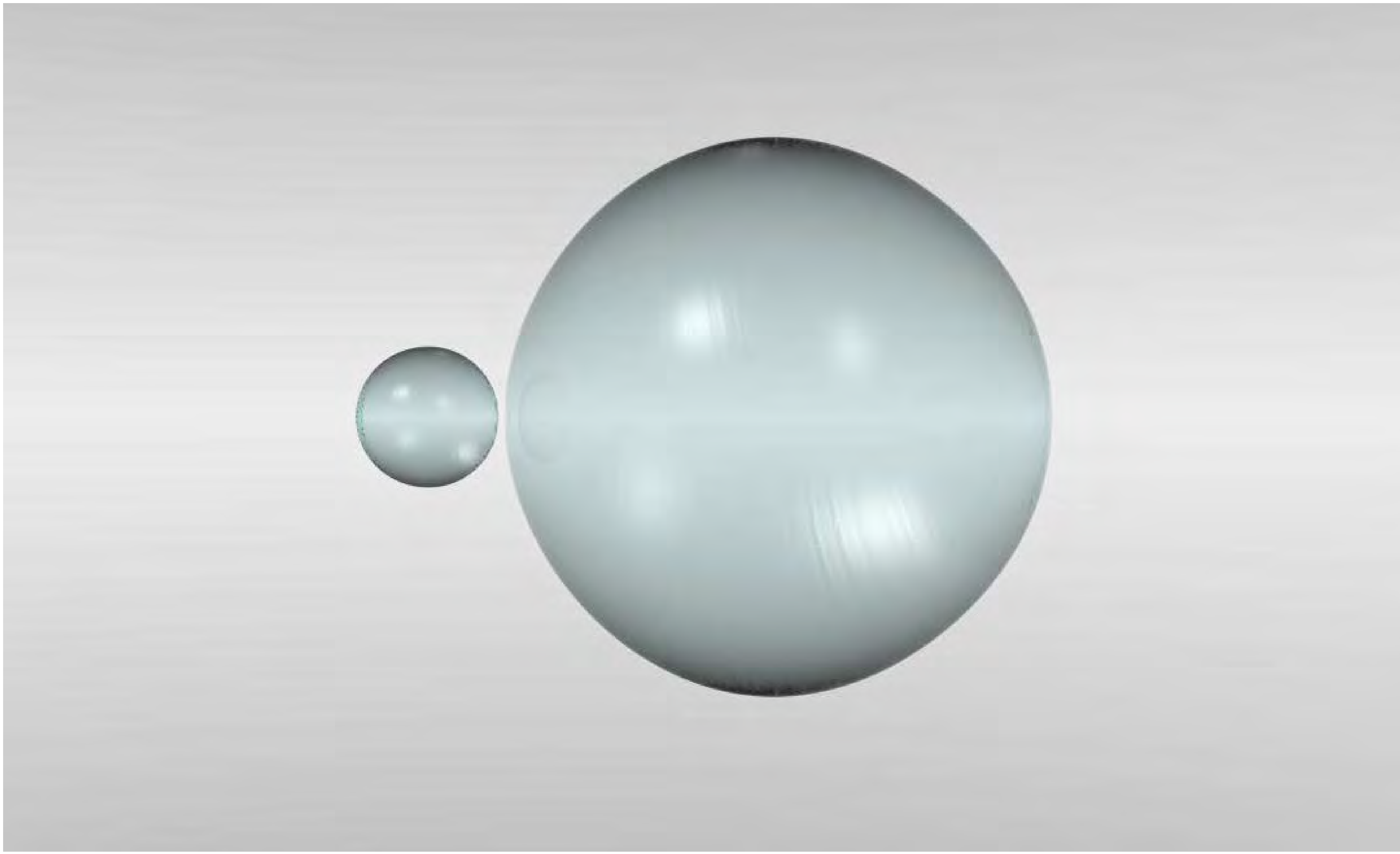






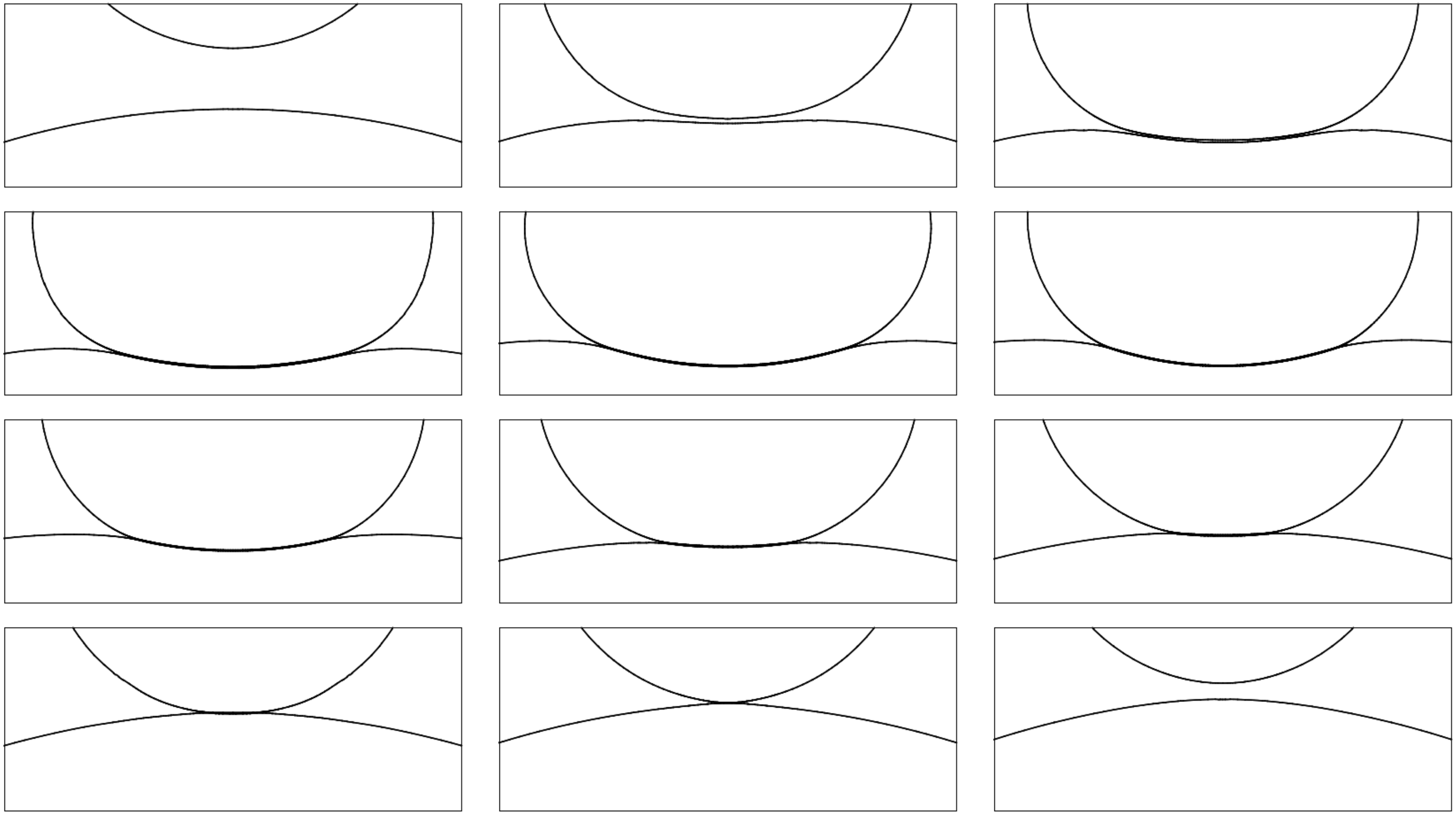






Unequal Bouncing (We = 1)

Droplet Diameter Ratio: 0.25



Conditions: water droplets in 1 atm. air, We=1, Re=85.2, B=0, Ds=100 μm, U=0.85 m/s.

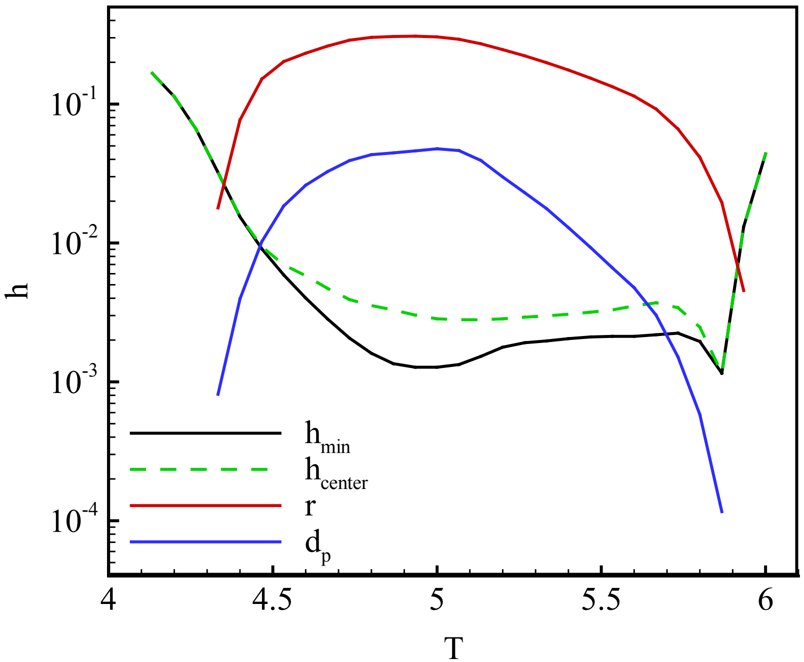
Georgia Tech

Shape Evolution

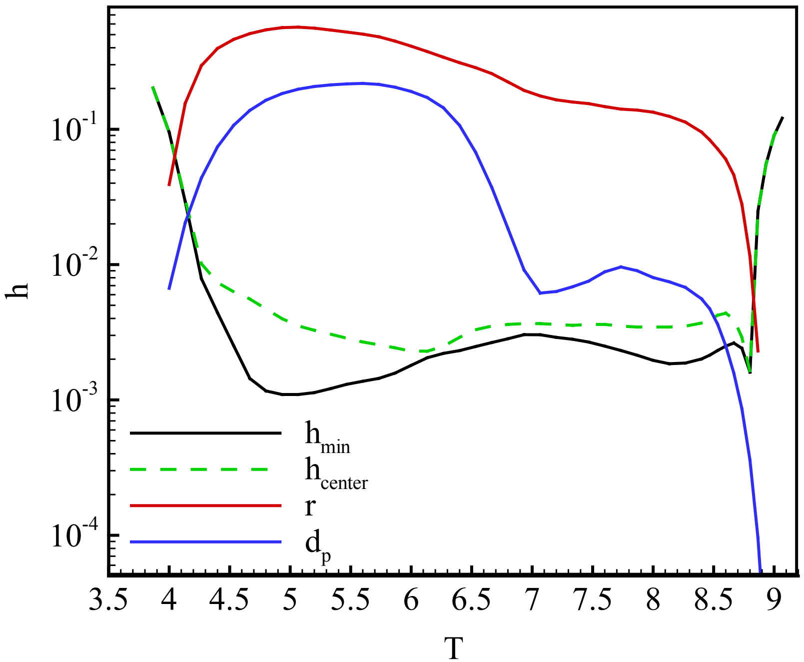
Droplet Diameter Ratio: 0.25

School of Aerospace Engineering

We = 1

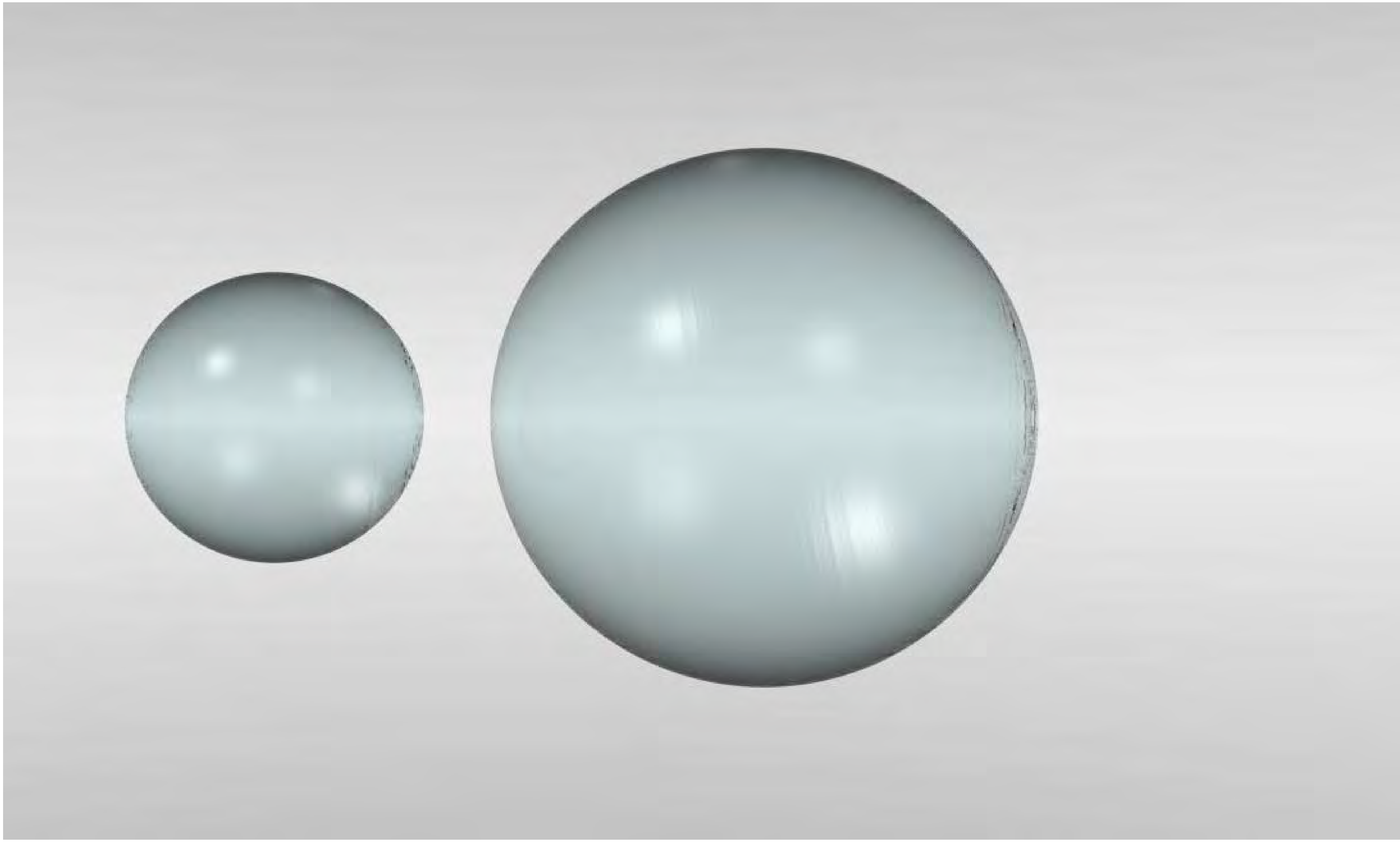


We = 10



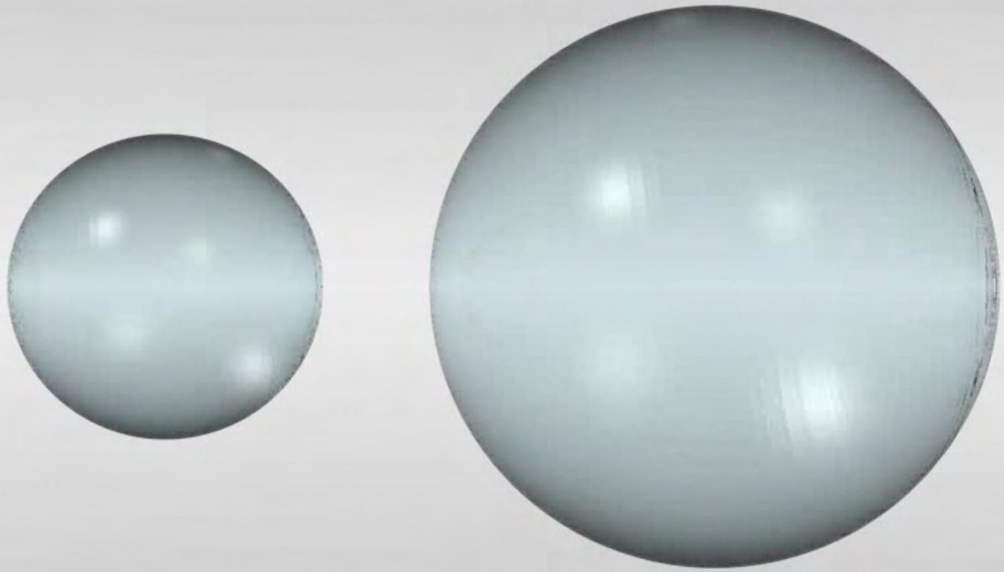
Unequal Bouncing (We = 10)

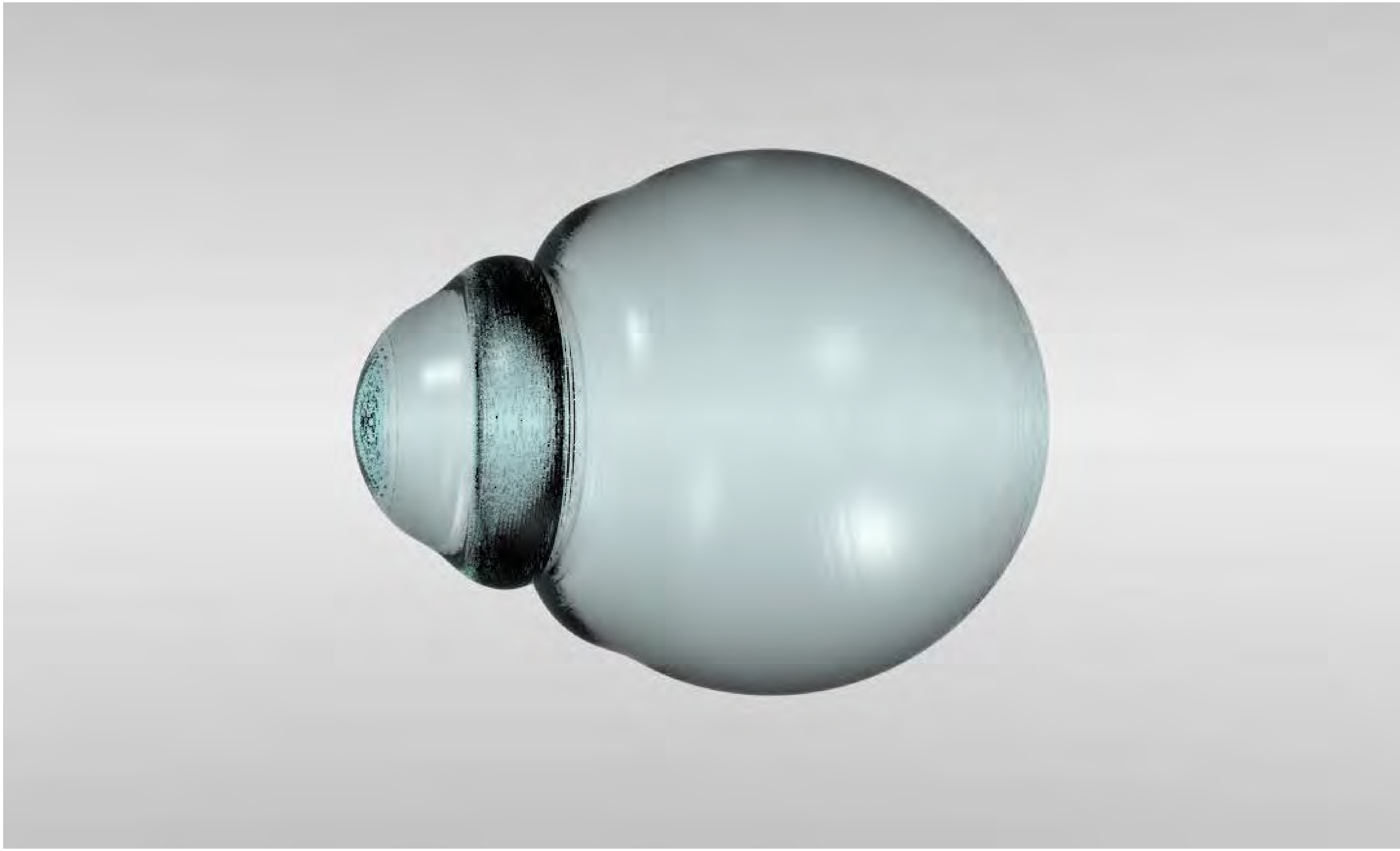
Droplet Diameter Ratio: 0.50

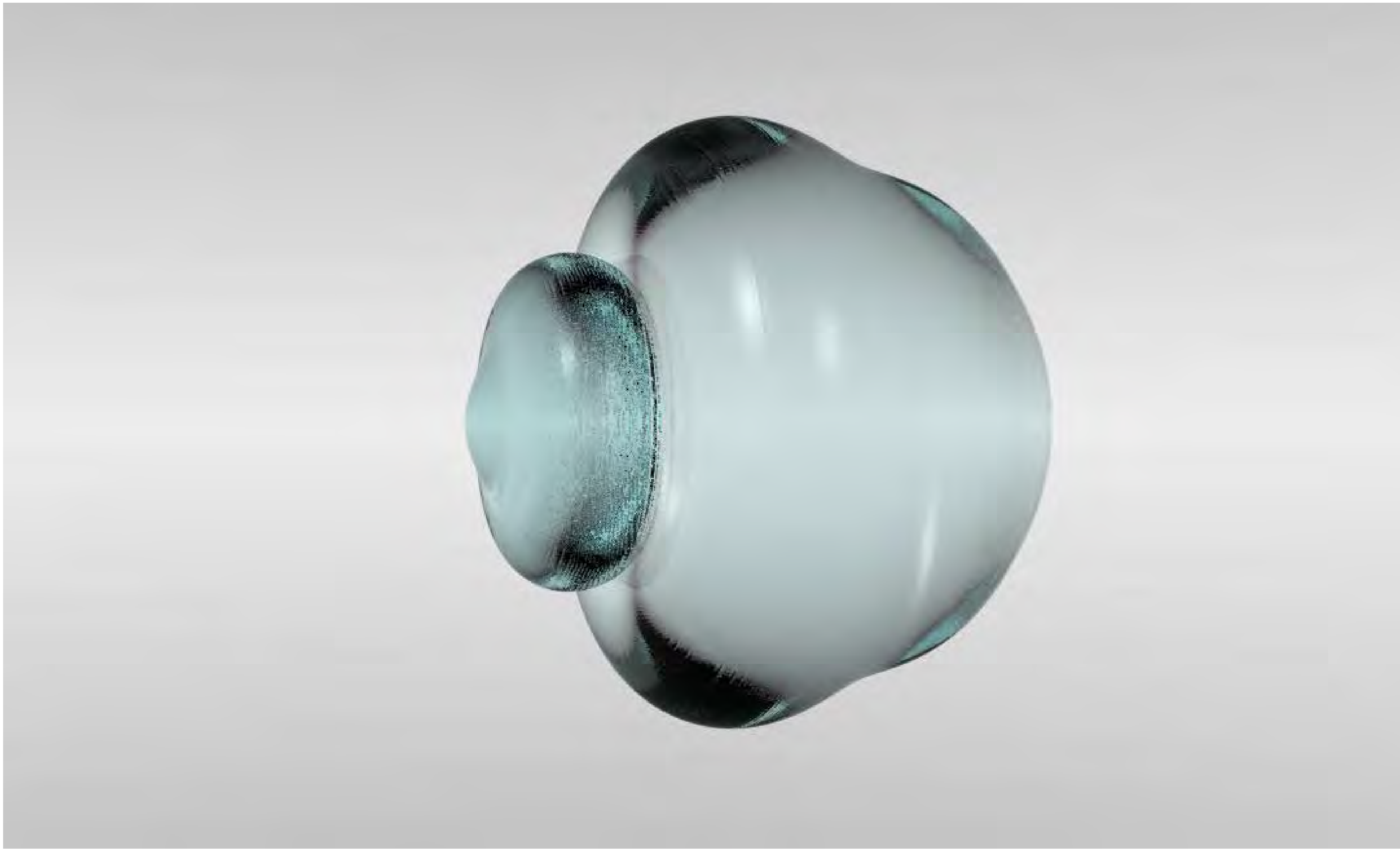


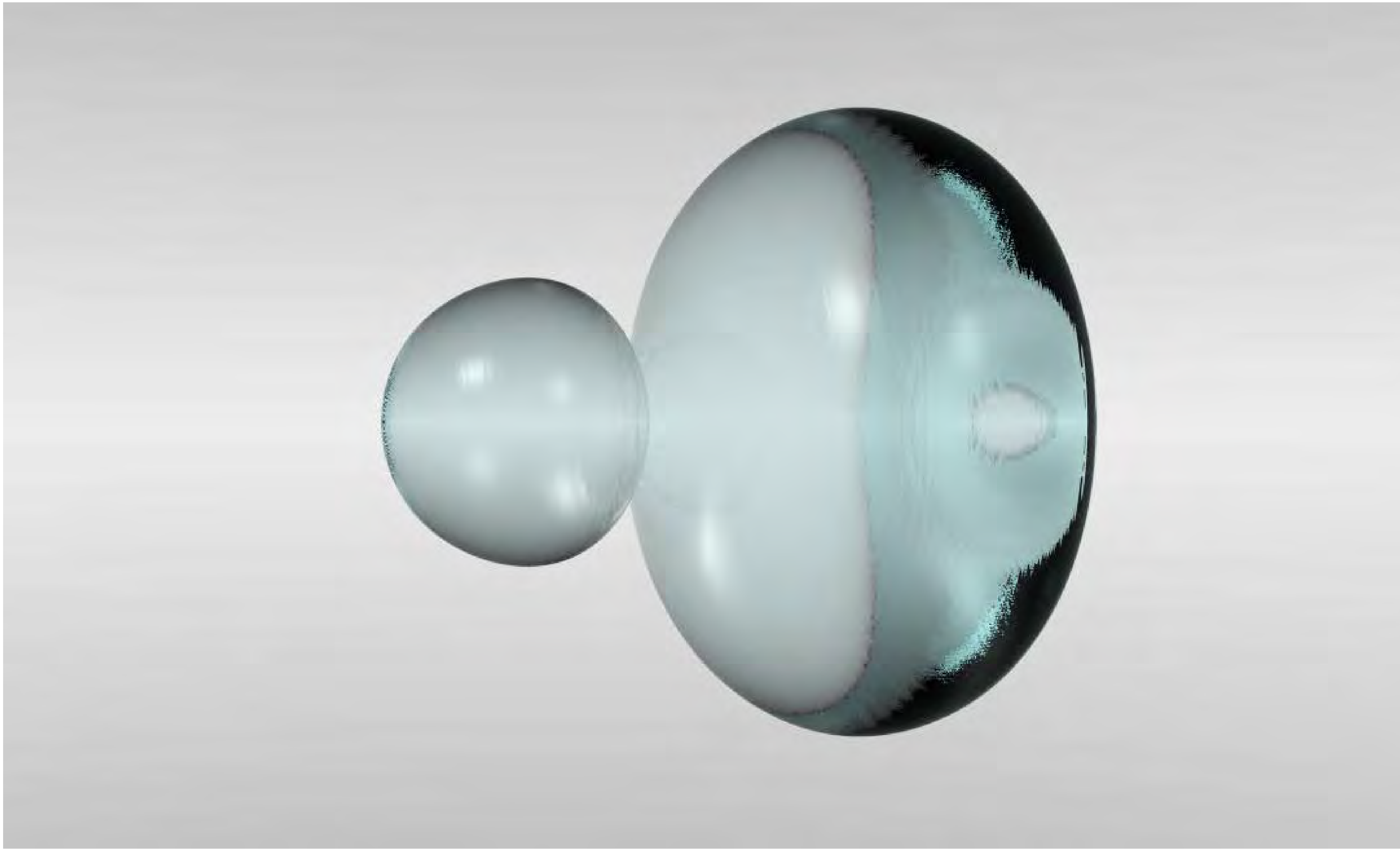
Conditions: water droplets in 1 atm. air, We=10, Re=377.6, B=0, Ds=200 μm, U=1.90 m/s

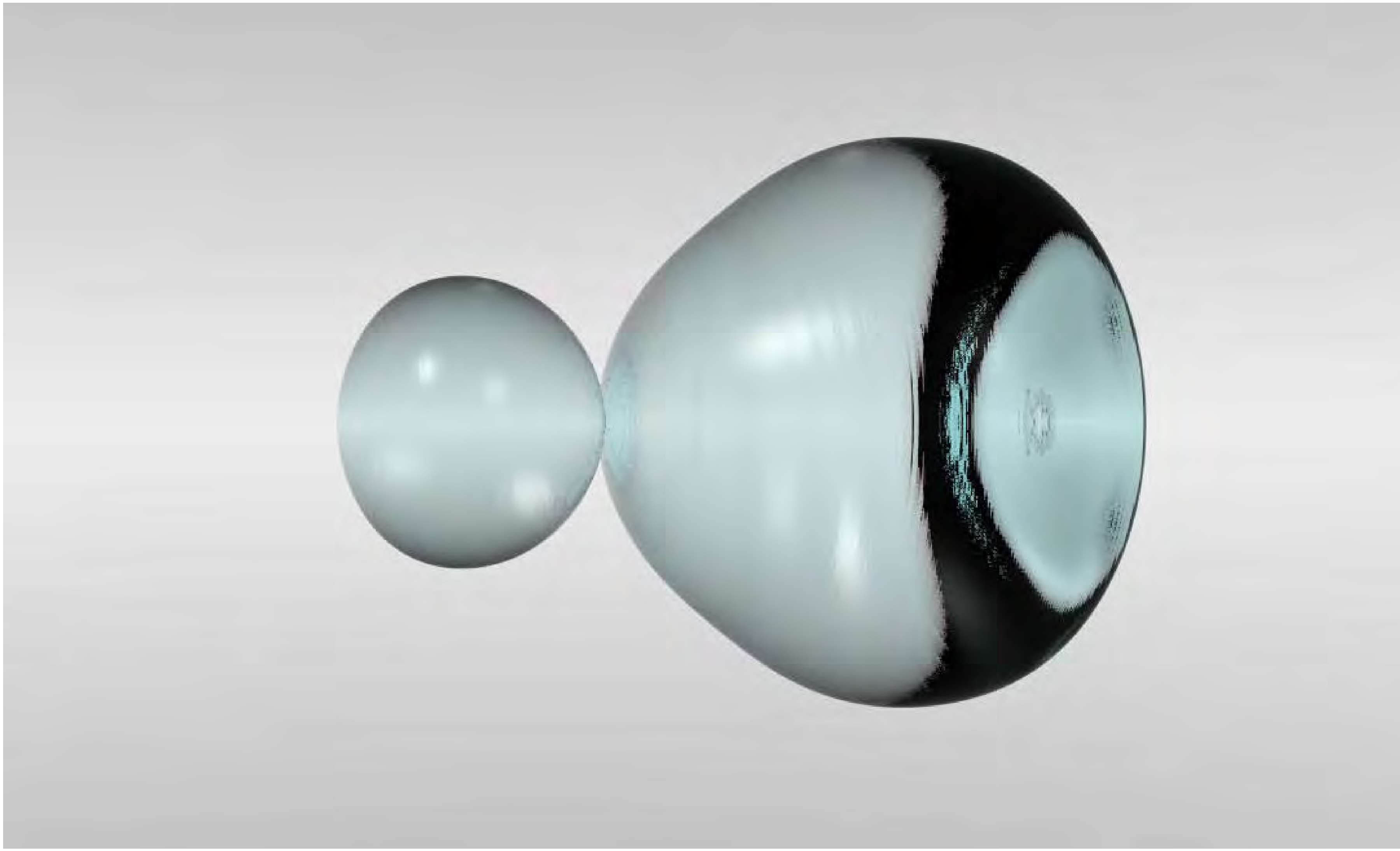
Movie

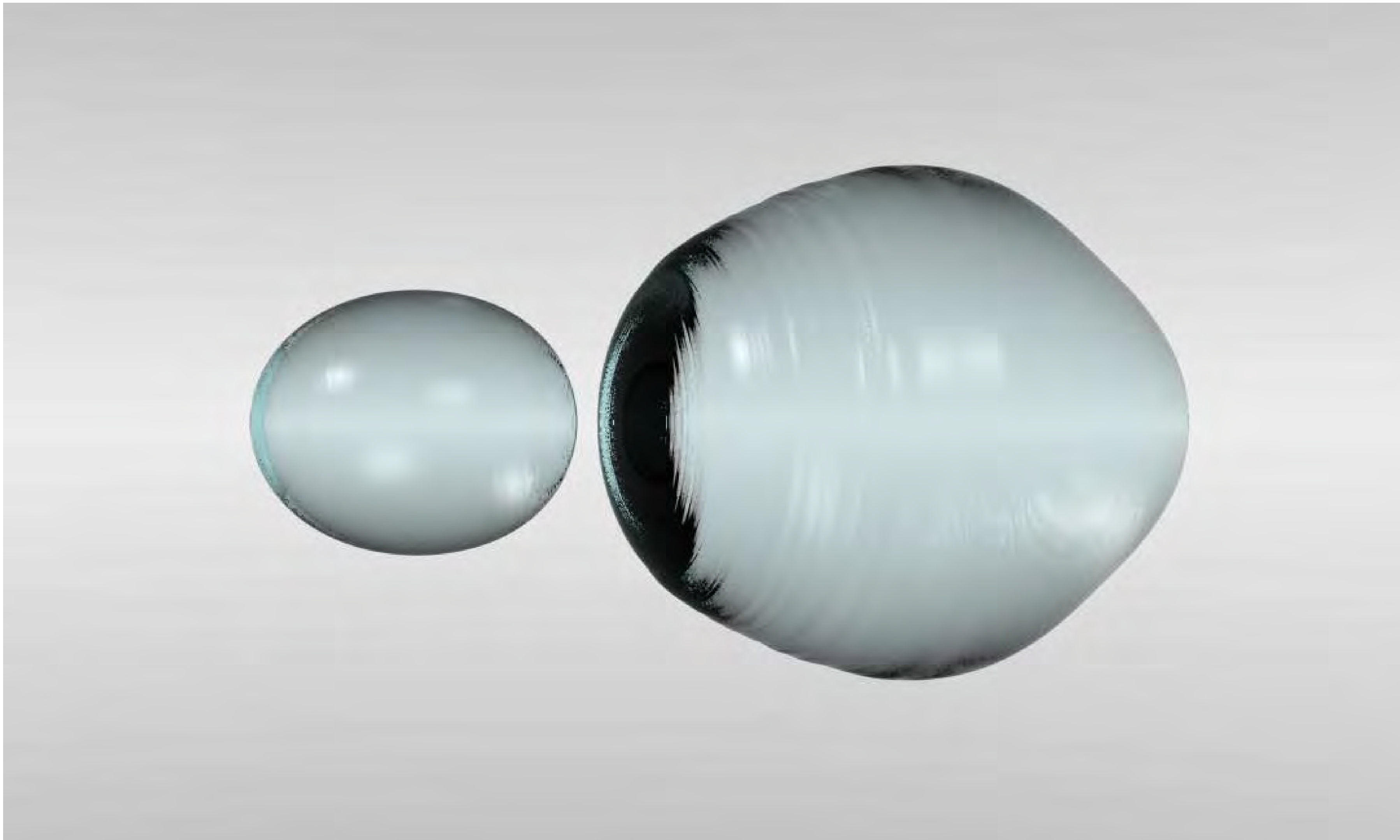


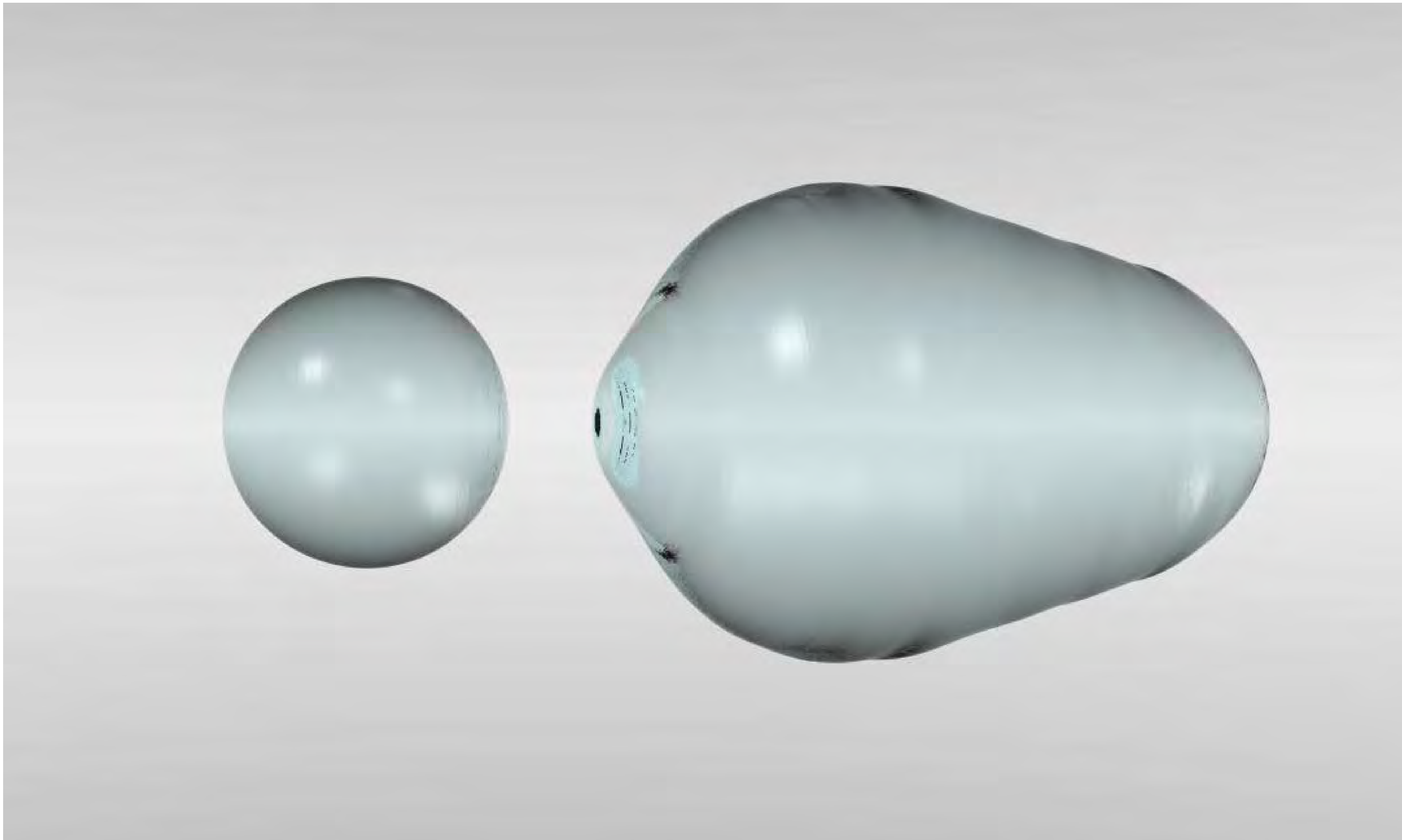


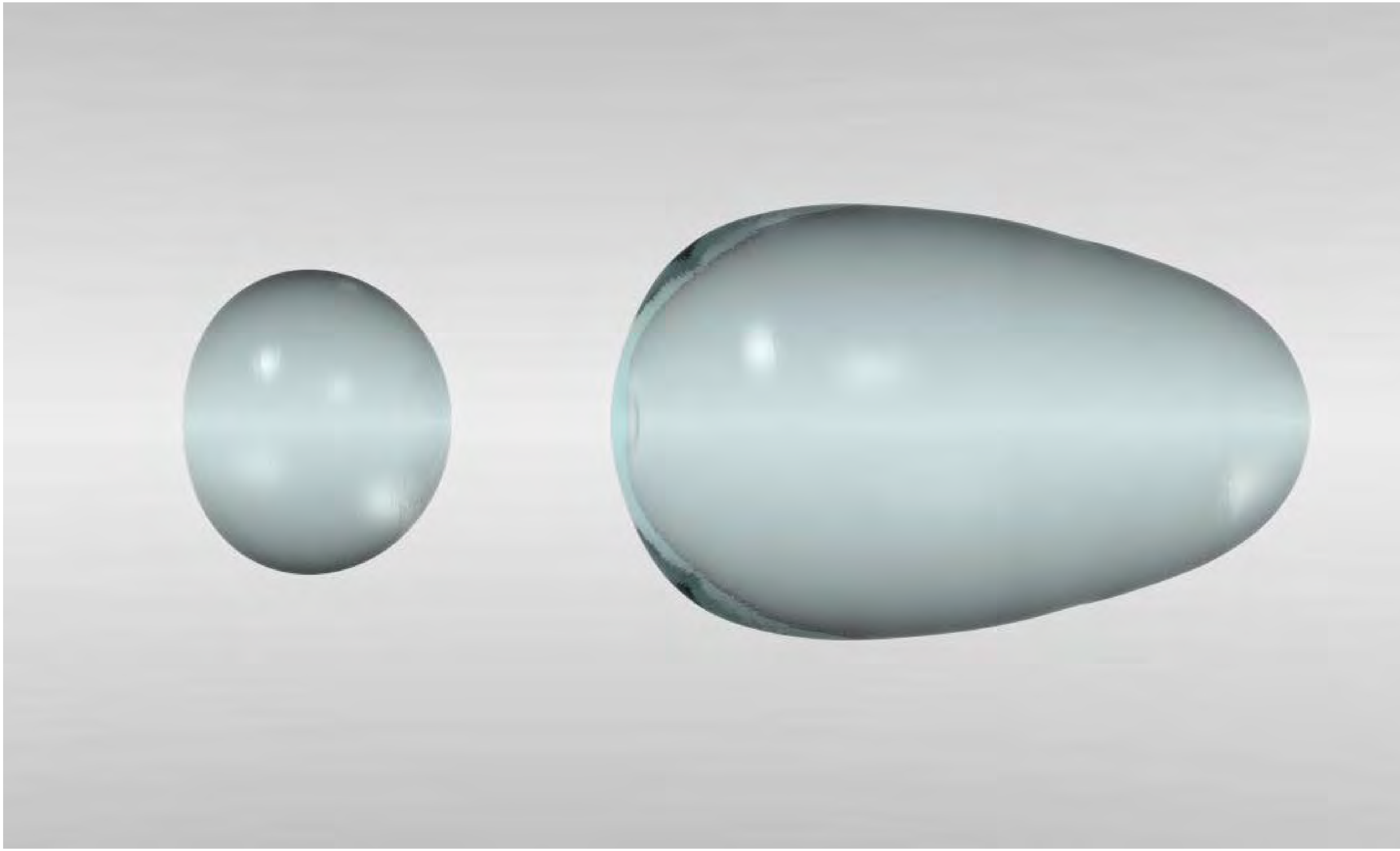






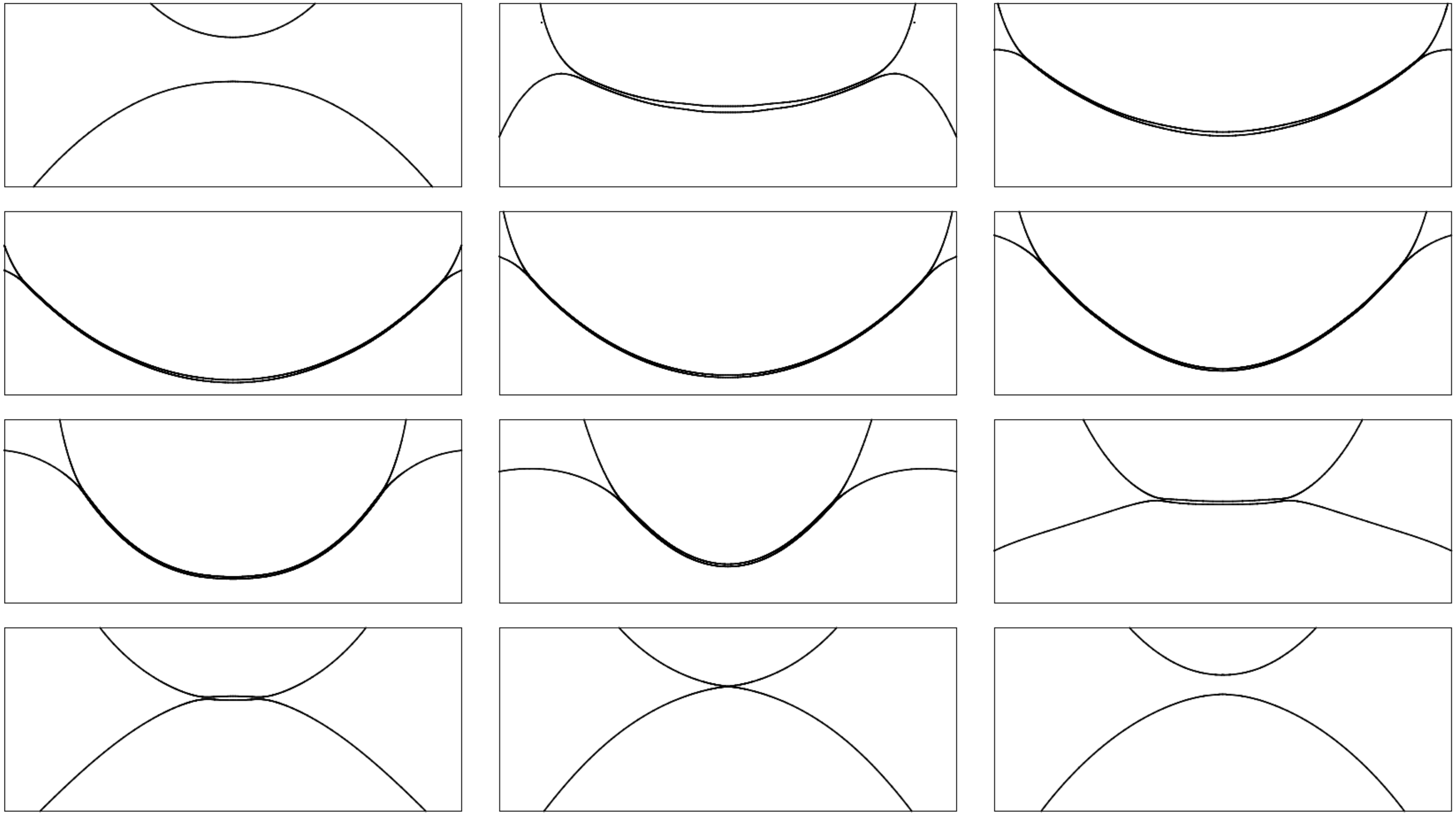






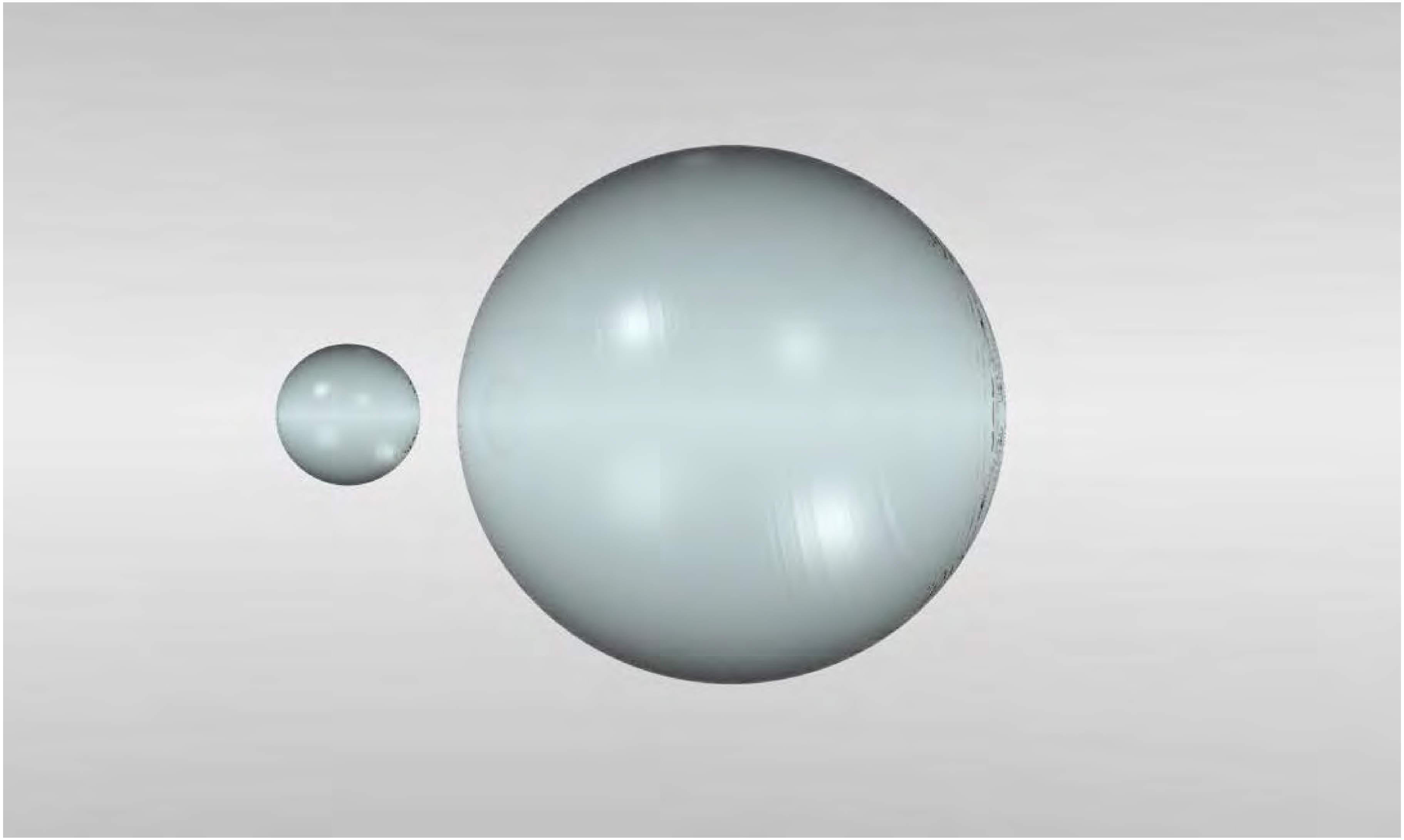
Unequal Bouncing (We = 10)

Droplet Diameter Ratio: 0.50



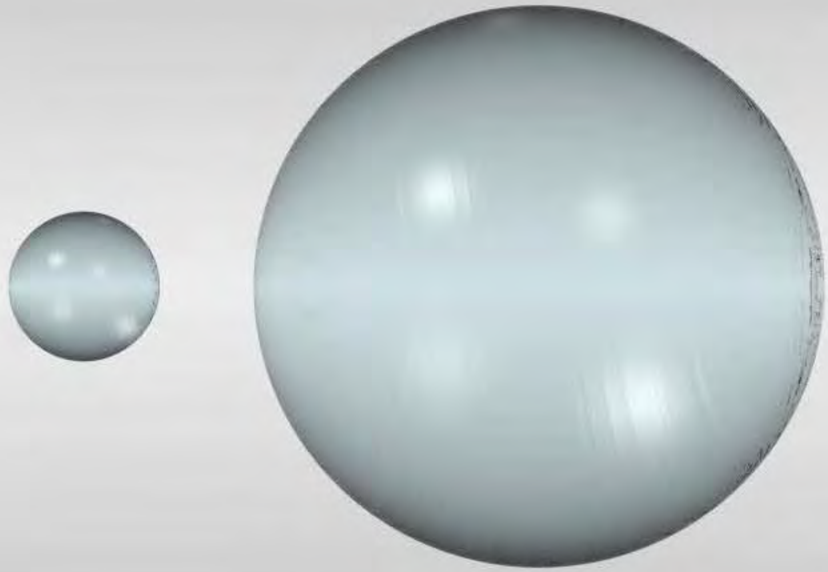
Conditions: water droplets in 1 atm. air, We=10, Re=377.6, B=0, Ds=200 μm, U=1.90 m/s

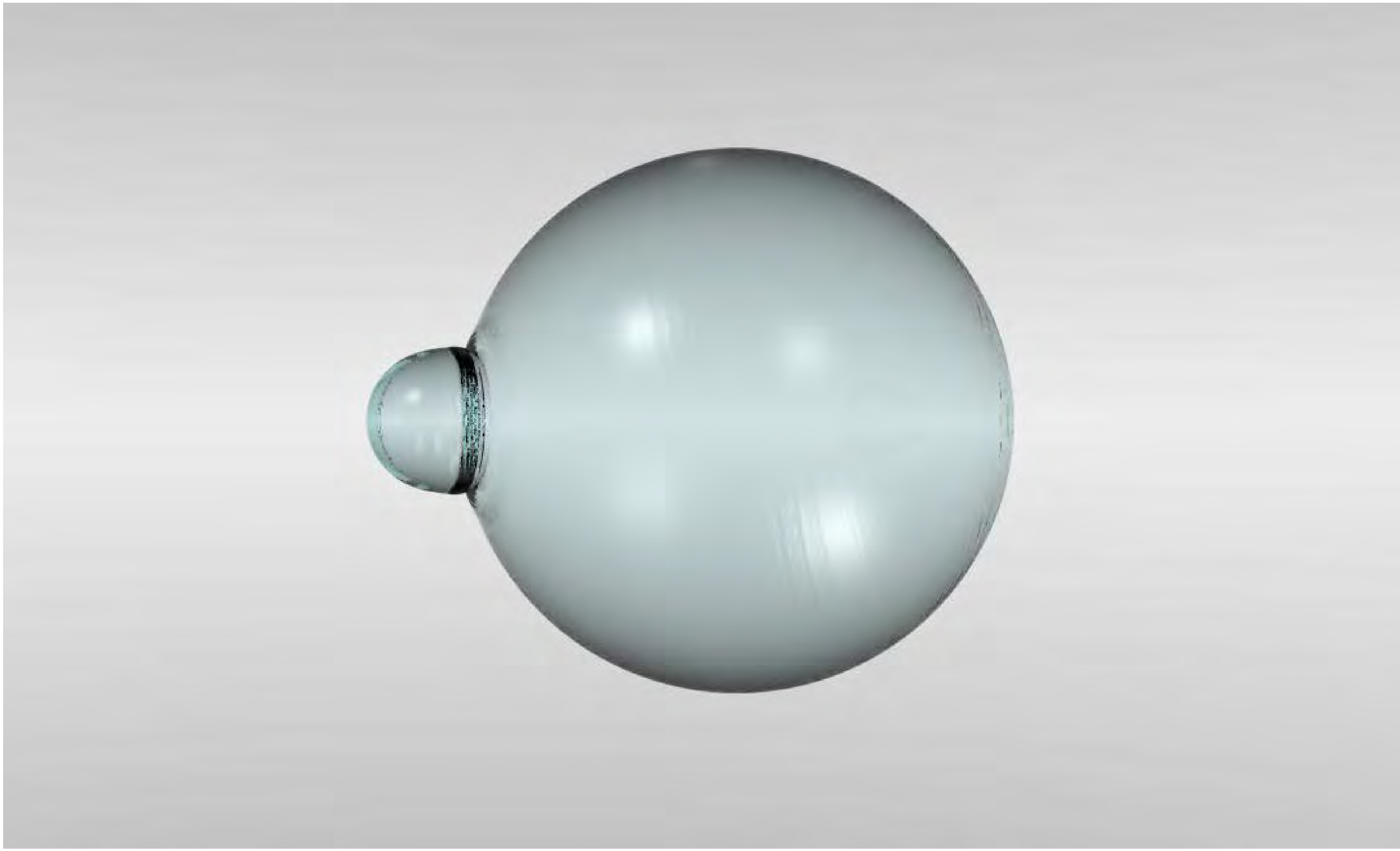
Unequal Bouncing (We = 10)
Droplet Diameter Ratio: 0.25

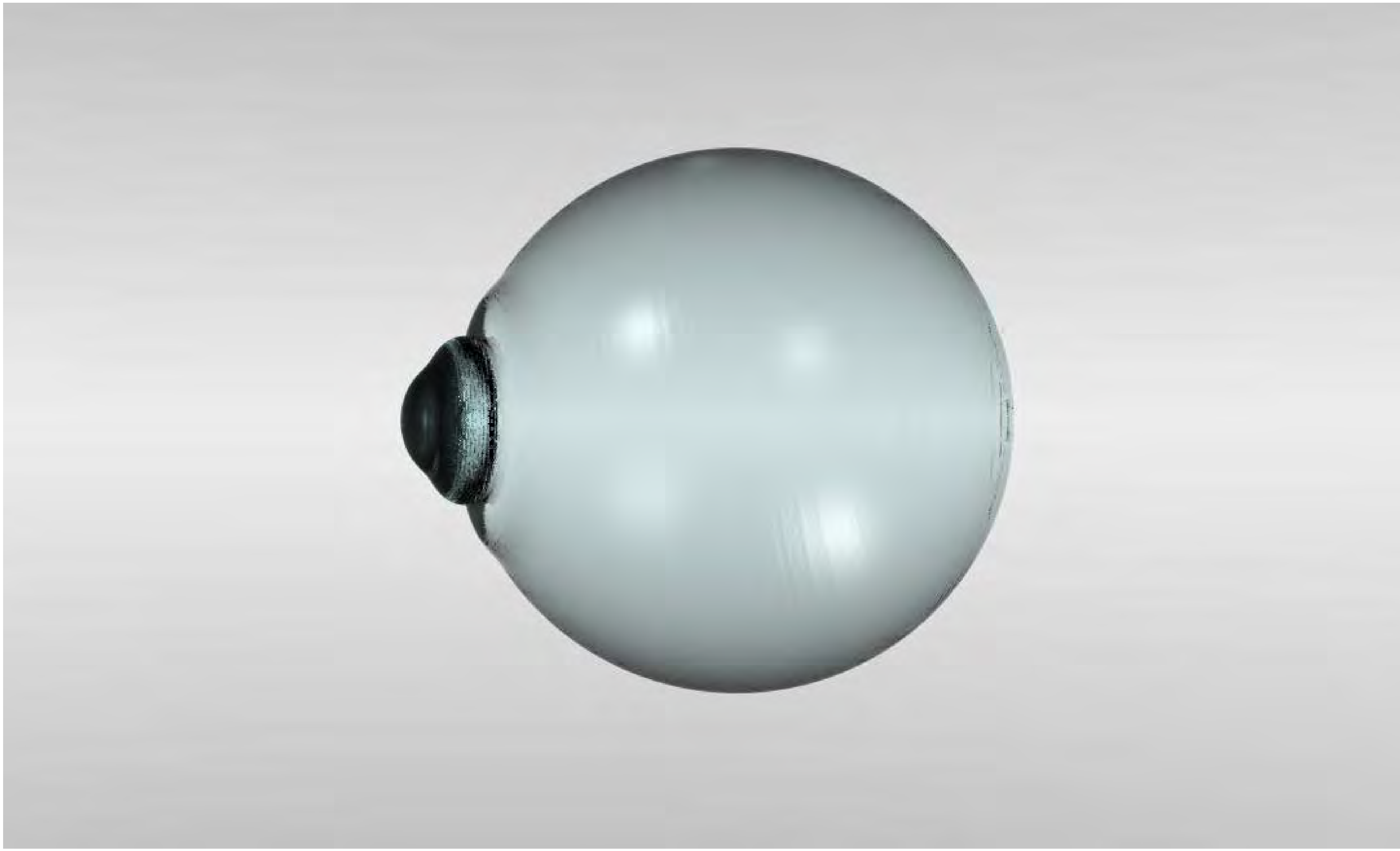


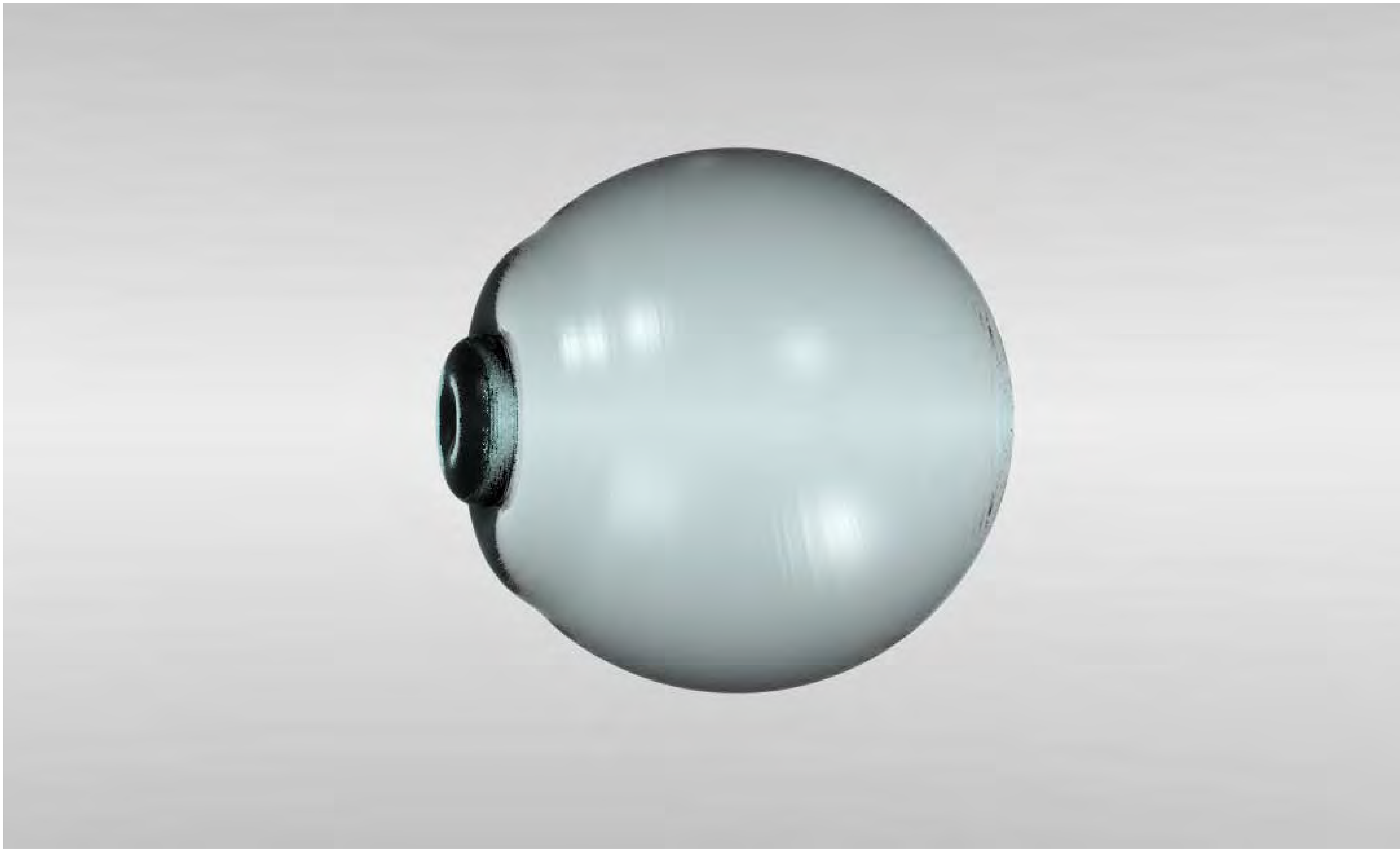
Conditions: water droplets in 1 atm. air, We=10, Re=269.4, B=0, Ds=100 μm, U=2.69 m/s.

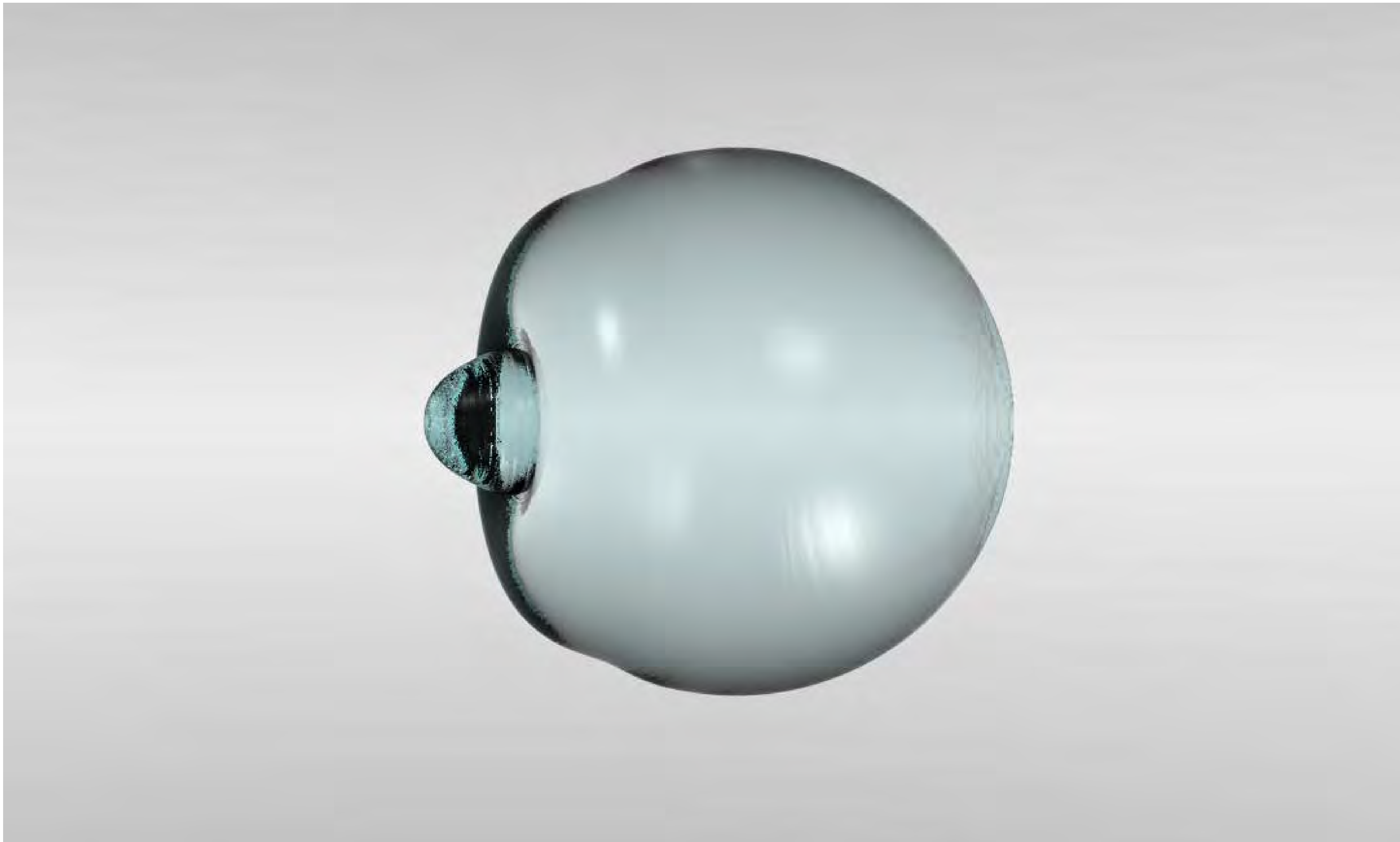
Movie

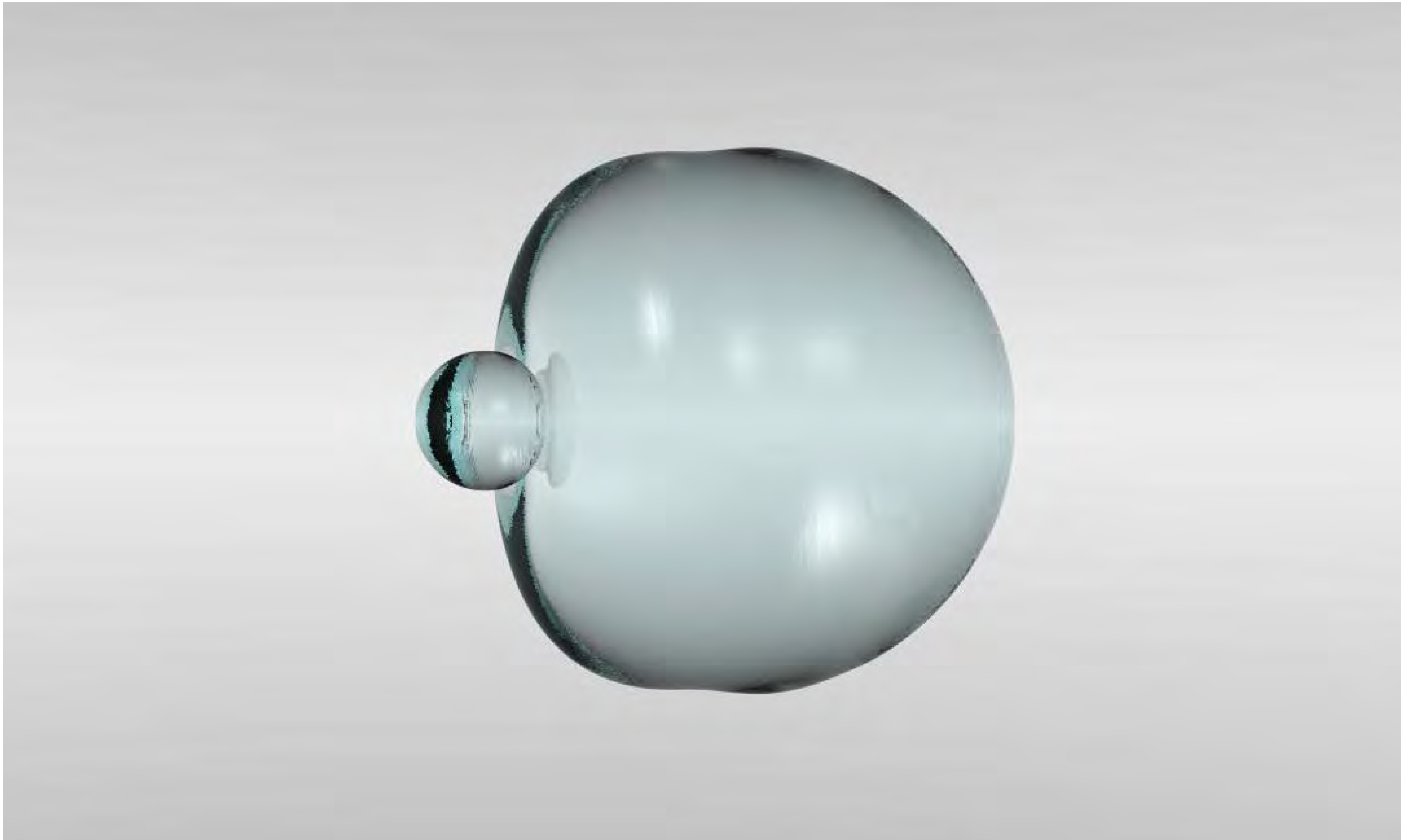


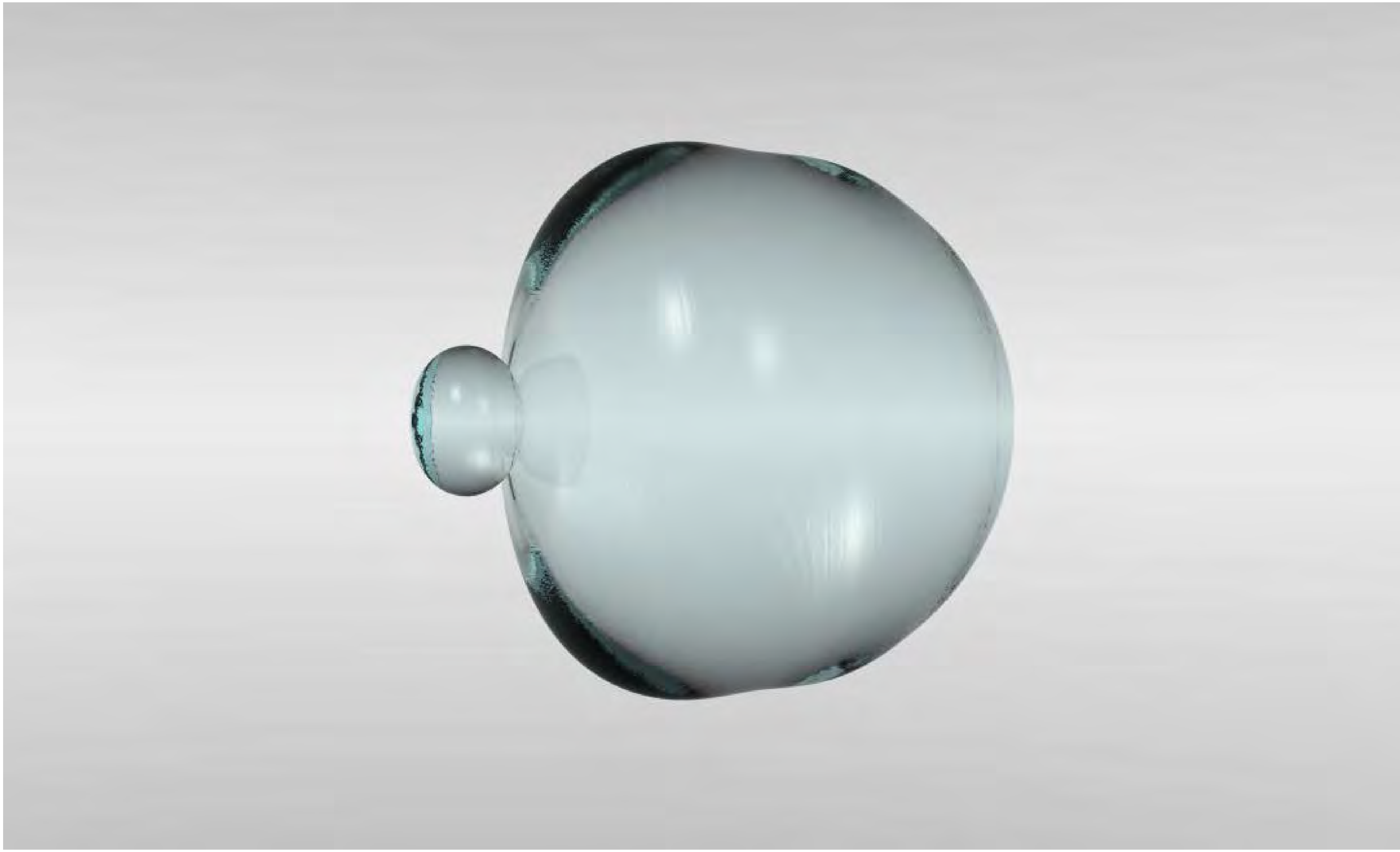


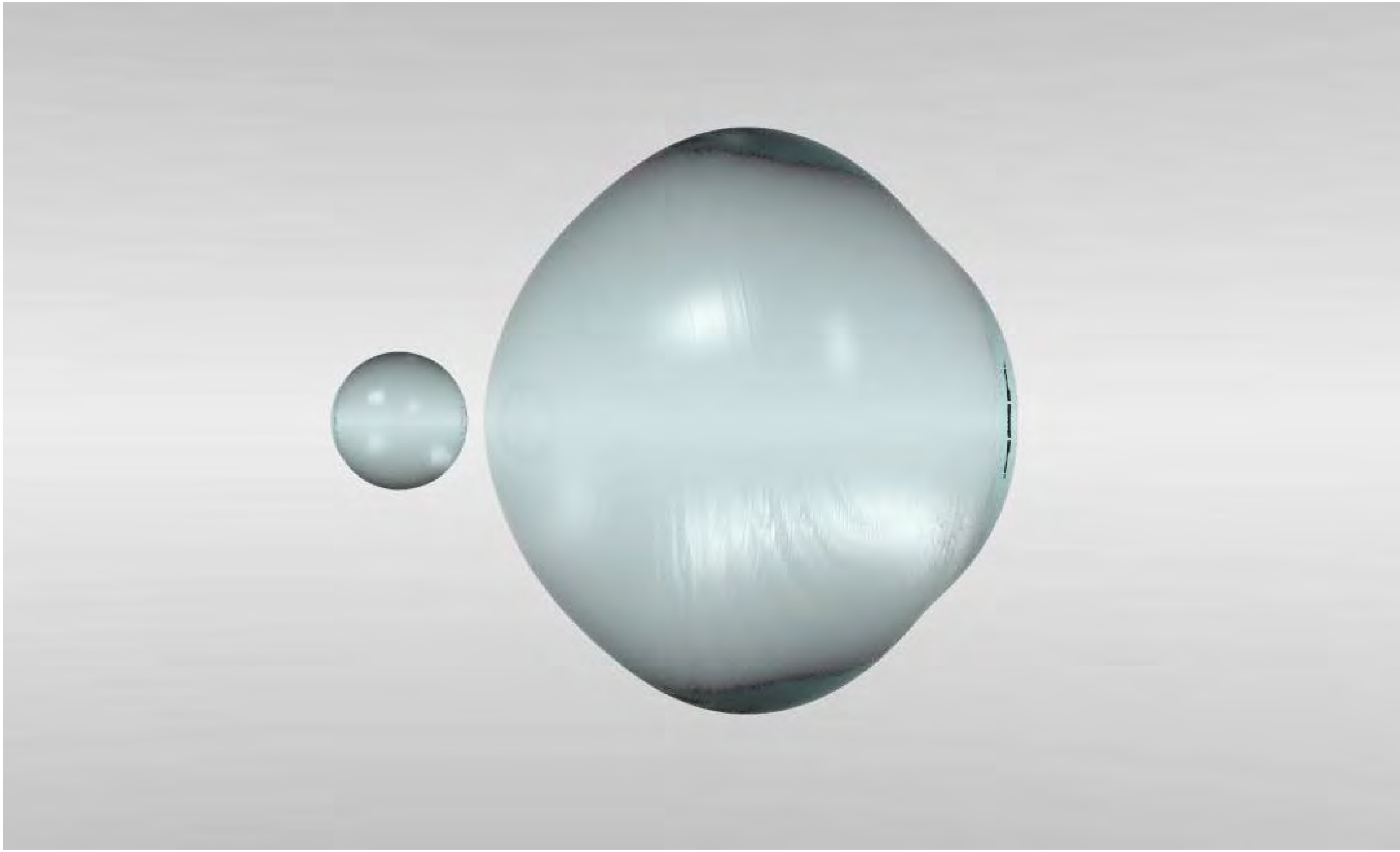






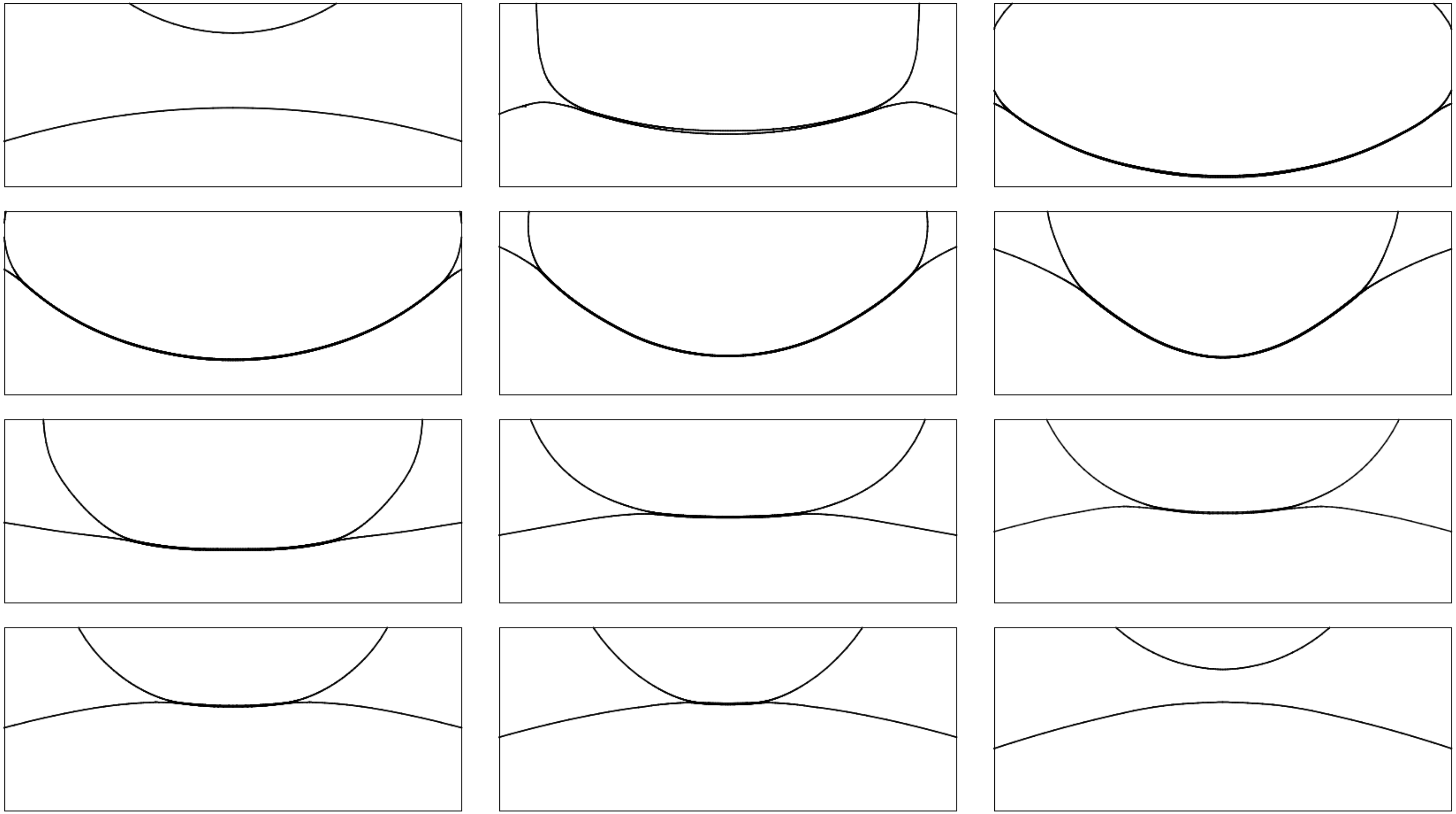






Unequal Bouncing (We = 10)

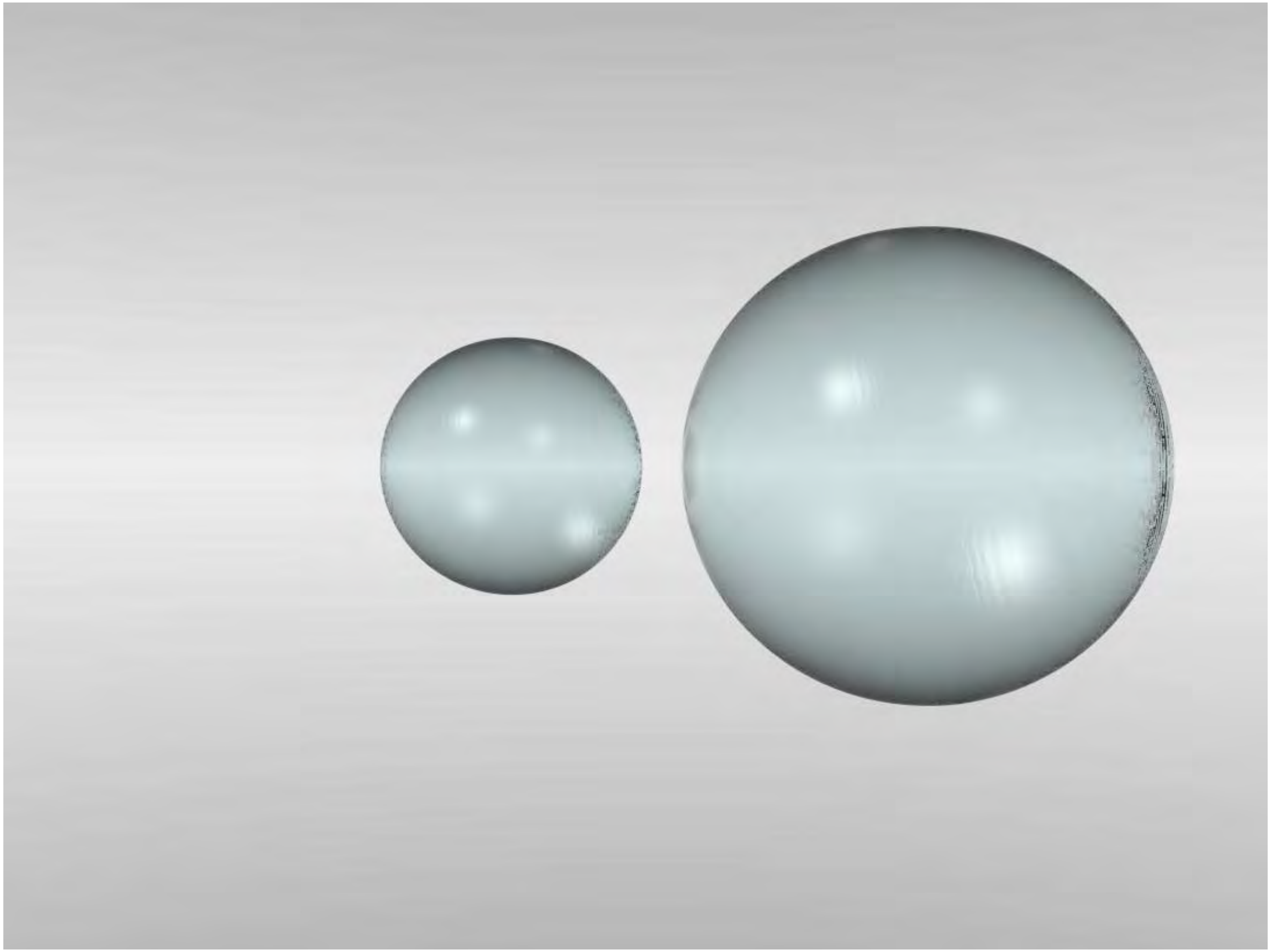
Droplet Diameter Ratio: 0.25



Conditions: water droplets in 1 atm. air, We=10, Re=269.4, B=0, Ds=100 μm, U=2.69 m/s.

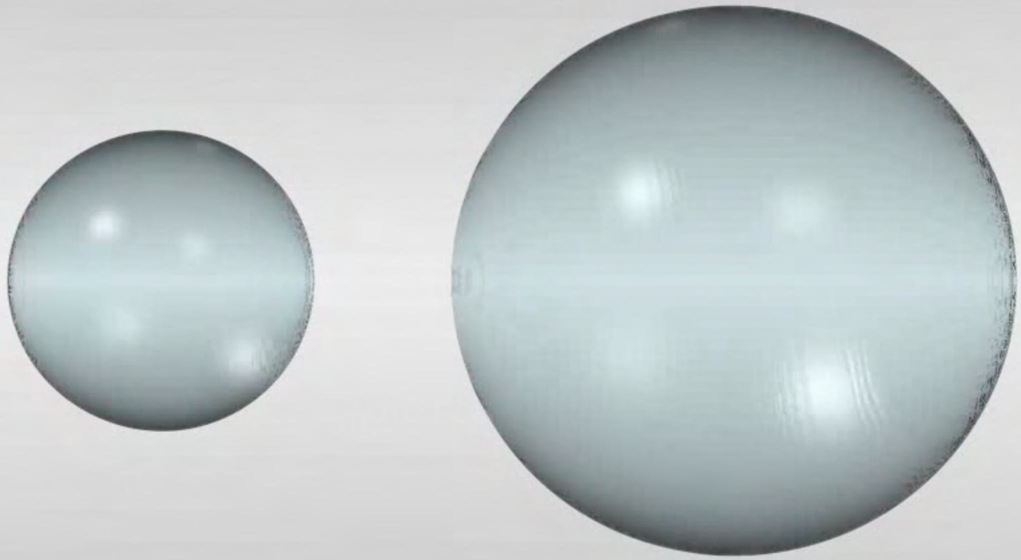
Unequal Merging (We = 100)

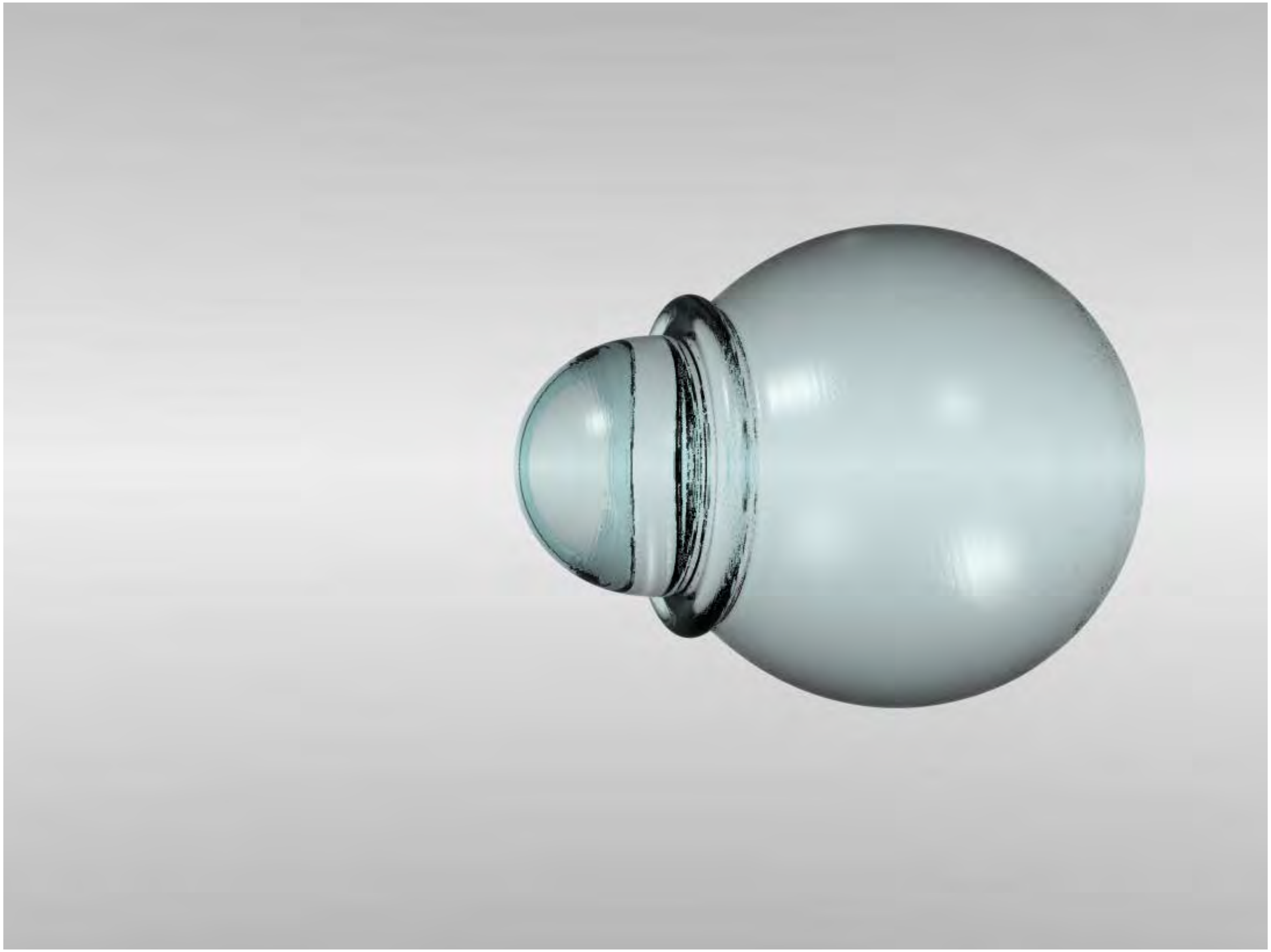
Droplet Diameter Ratio: 0.50

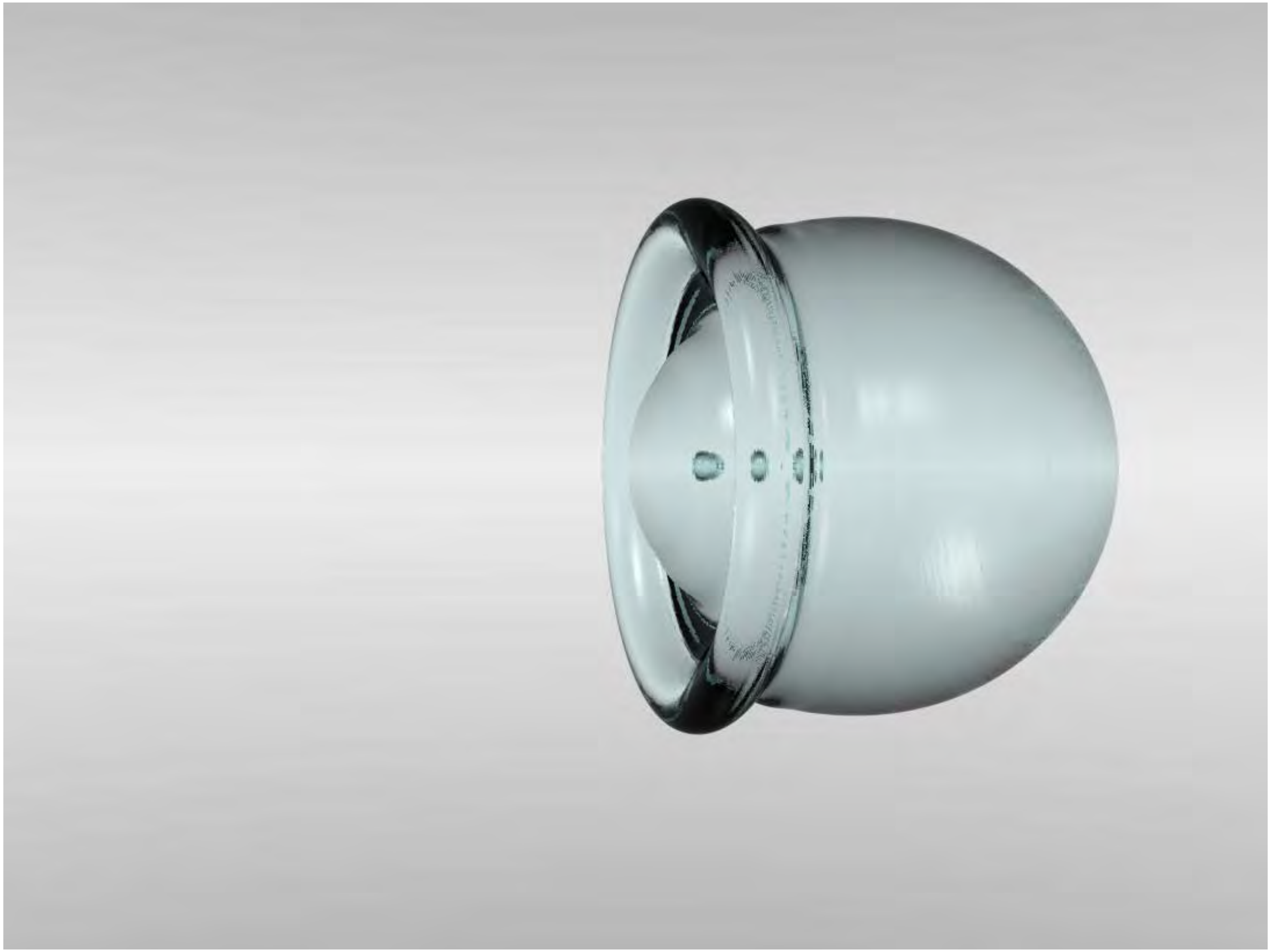


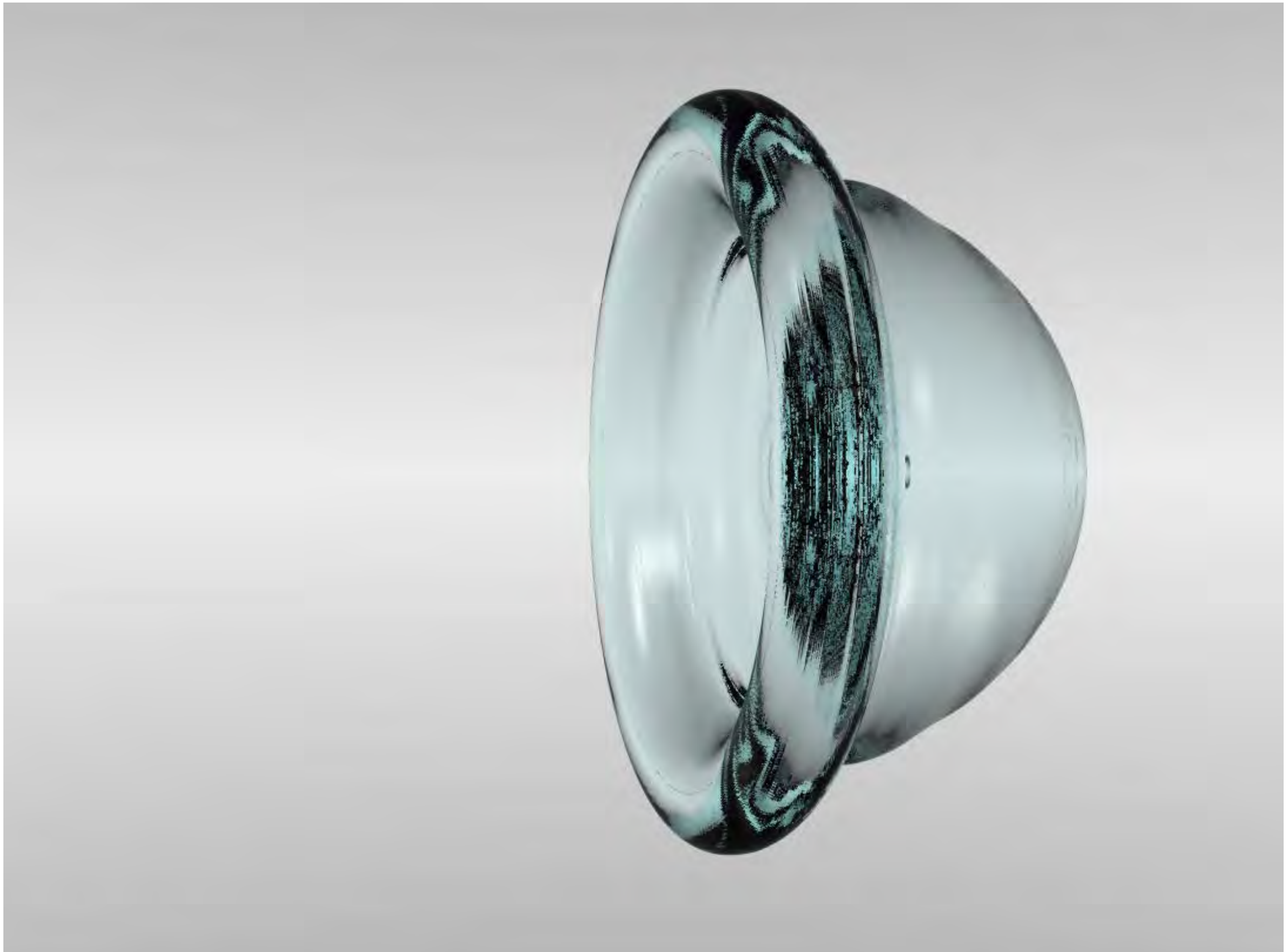
Conditions: water droplets in 1 atm. air, We=100, Re=1190.4, B=0, D_s=200 μm, U=6.0 m/s.

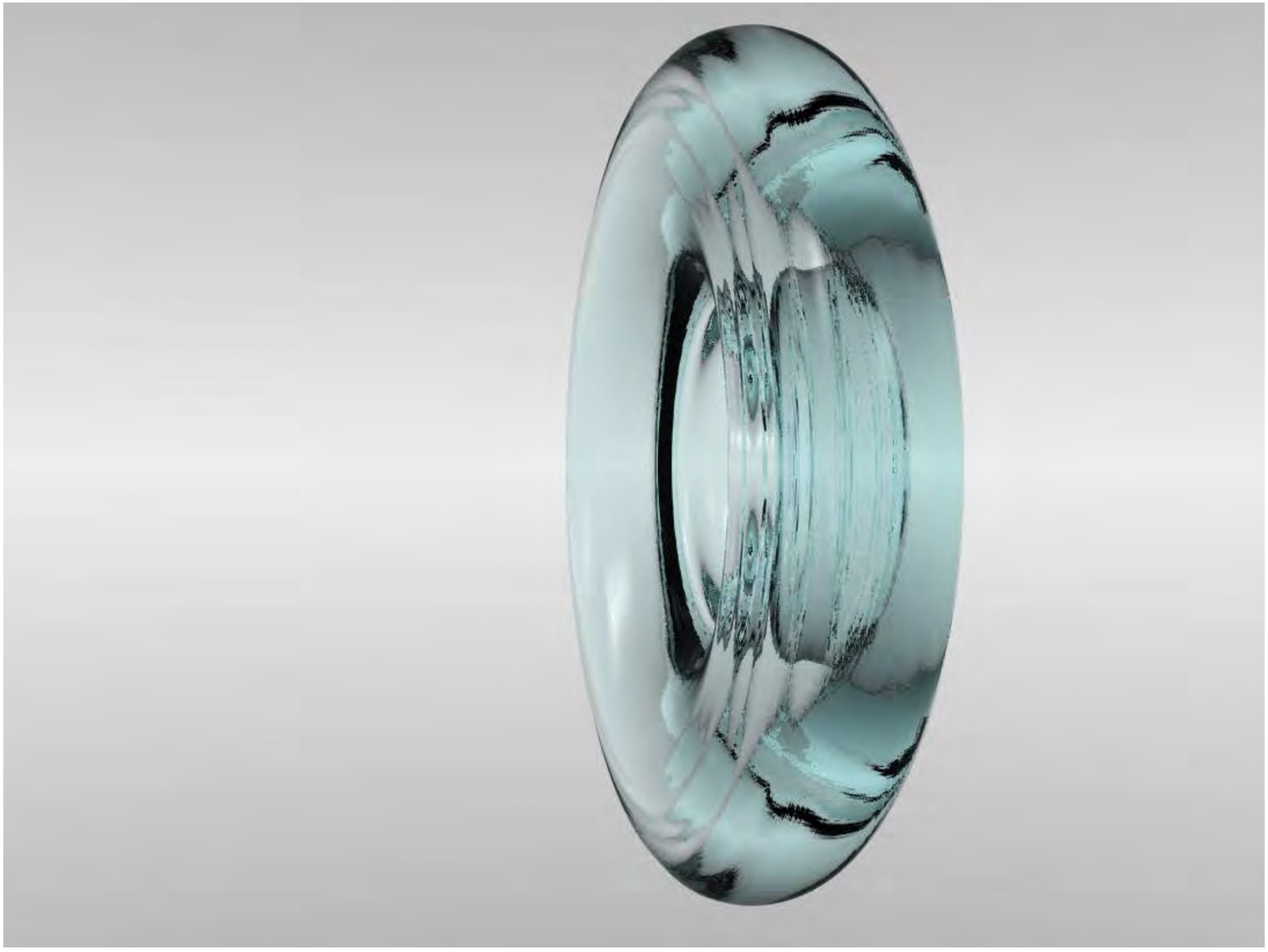
Movie

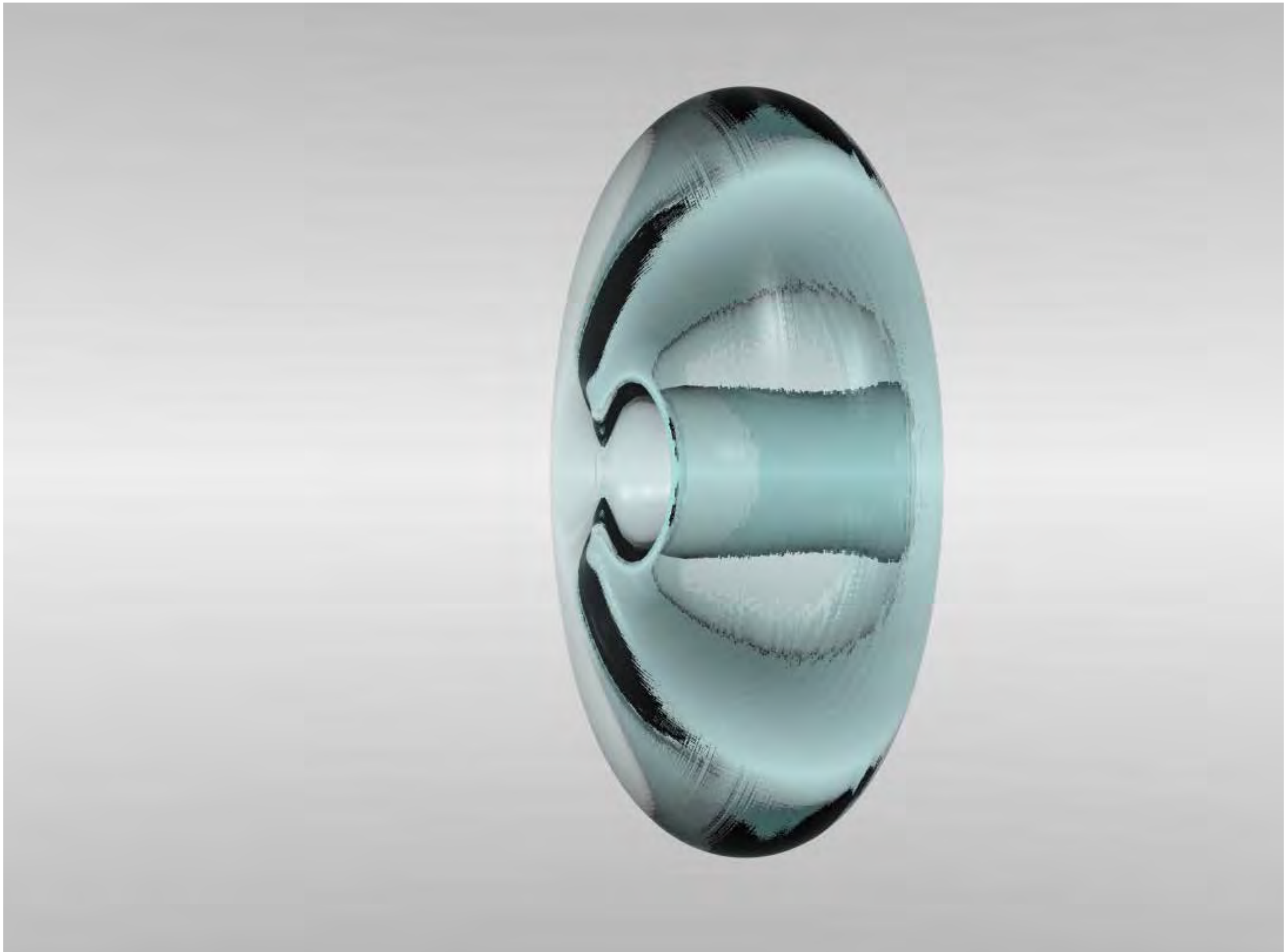


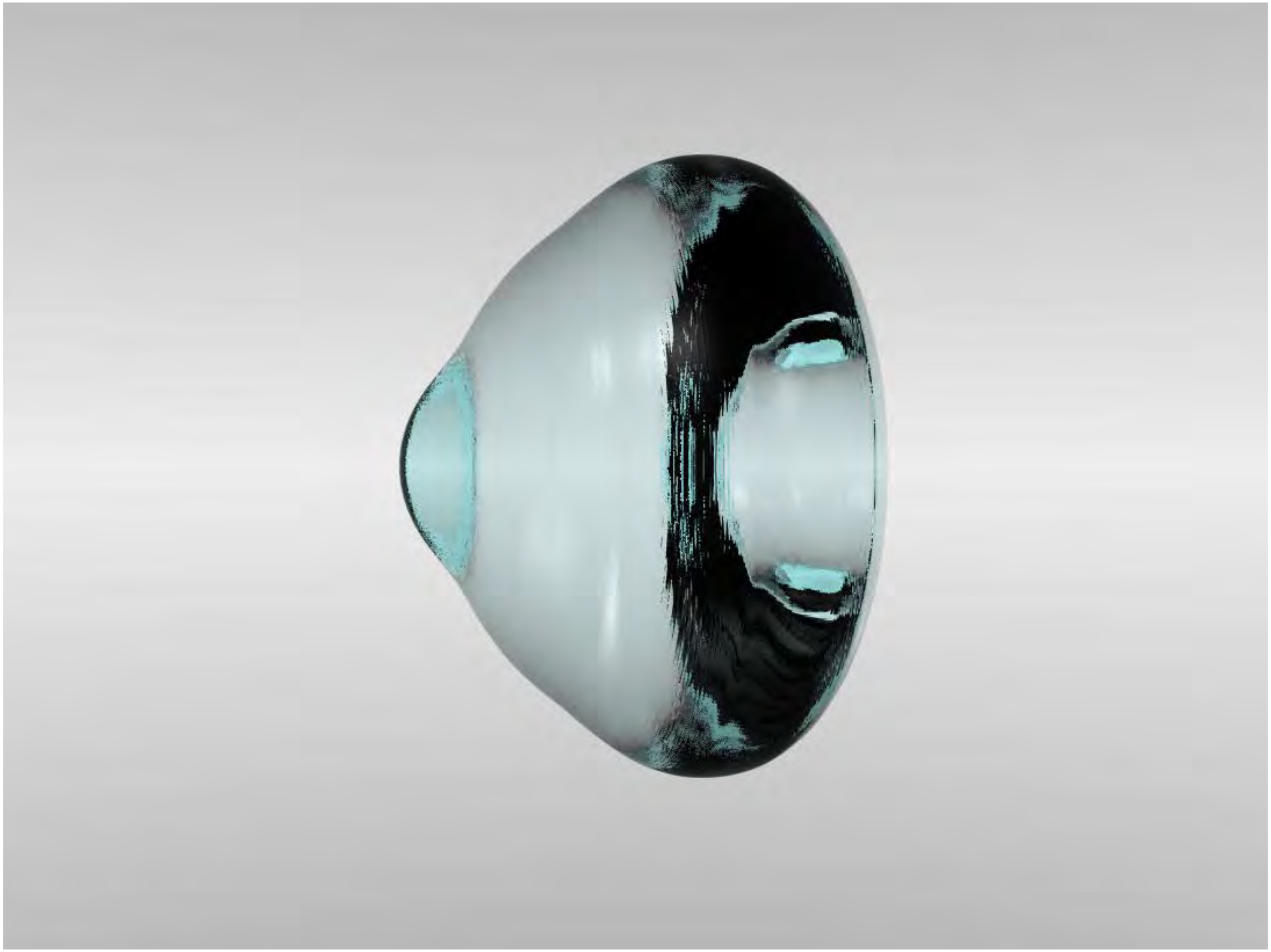


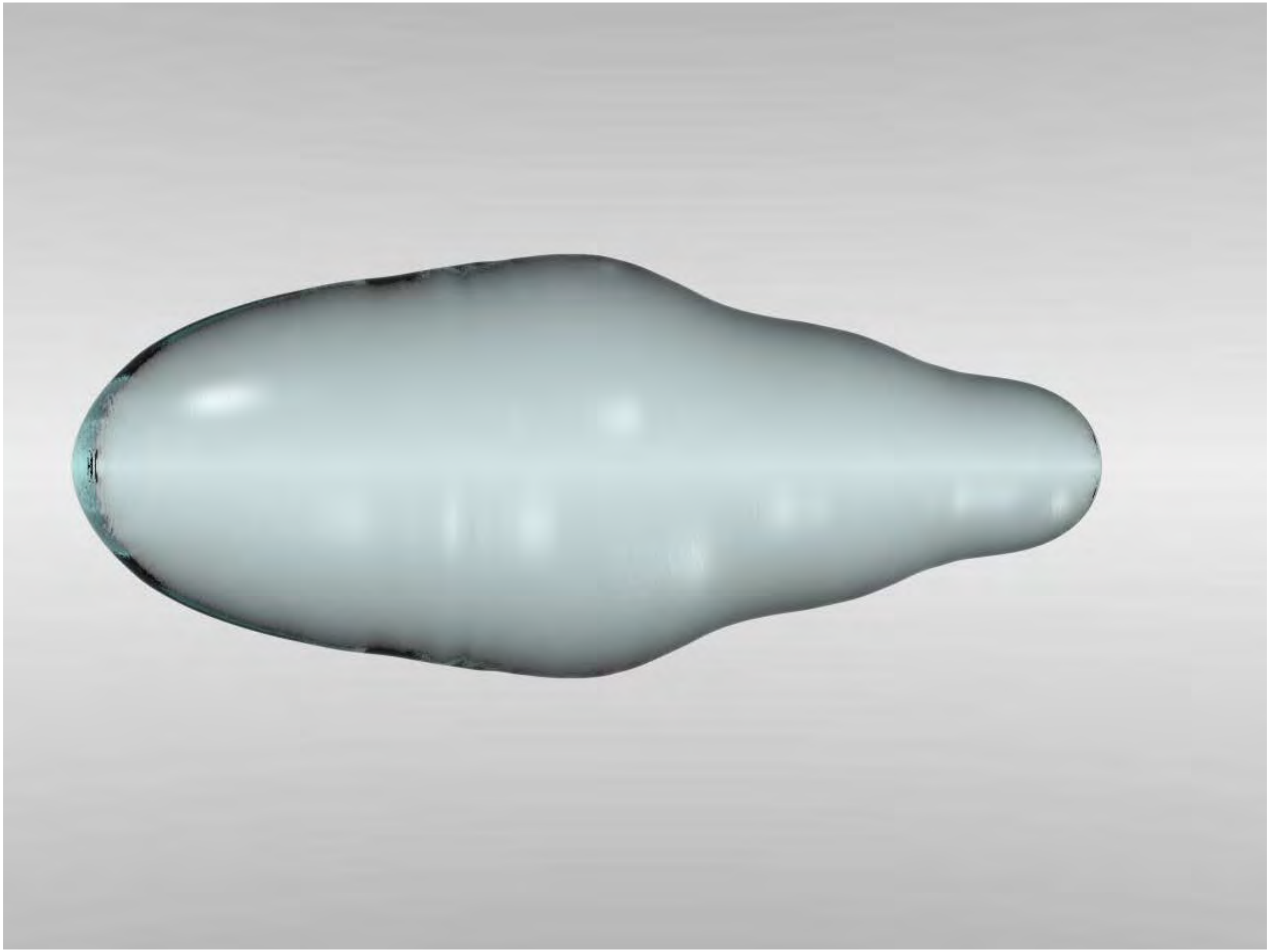






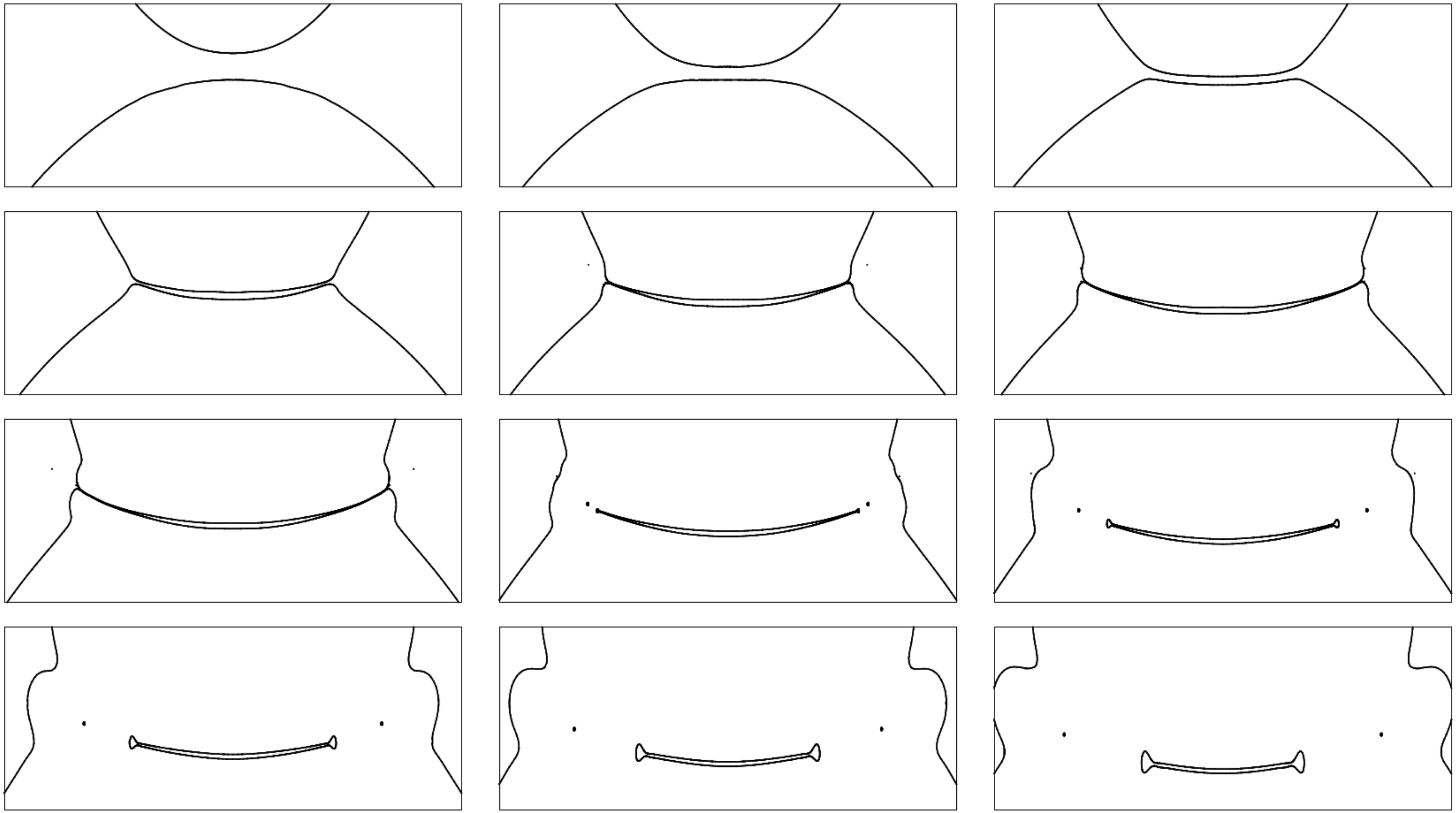






Unequal Merging (We = 100)

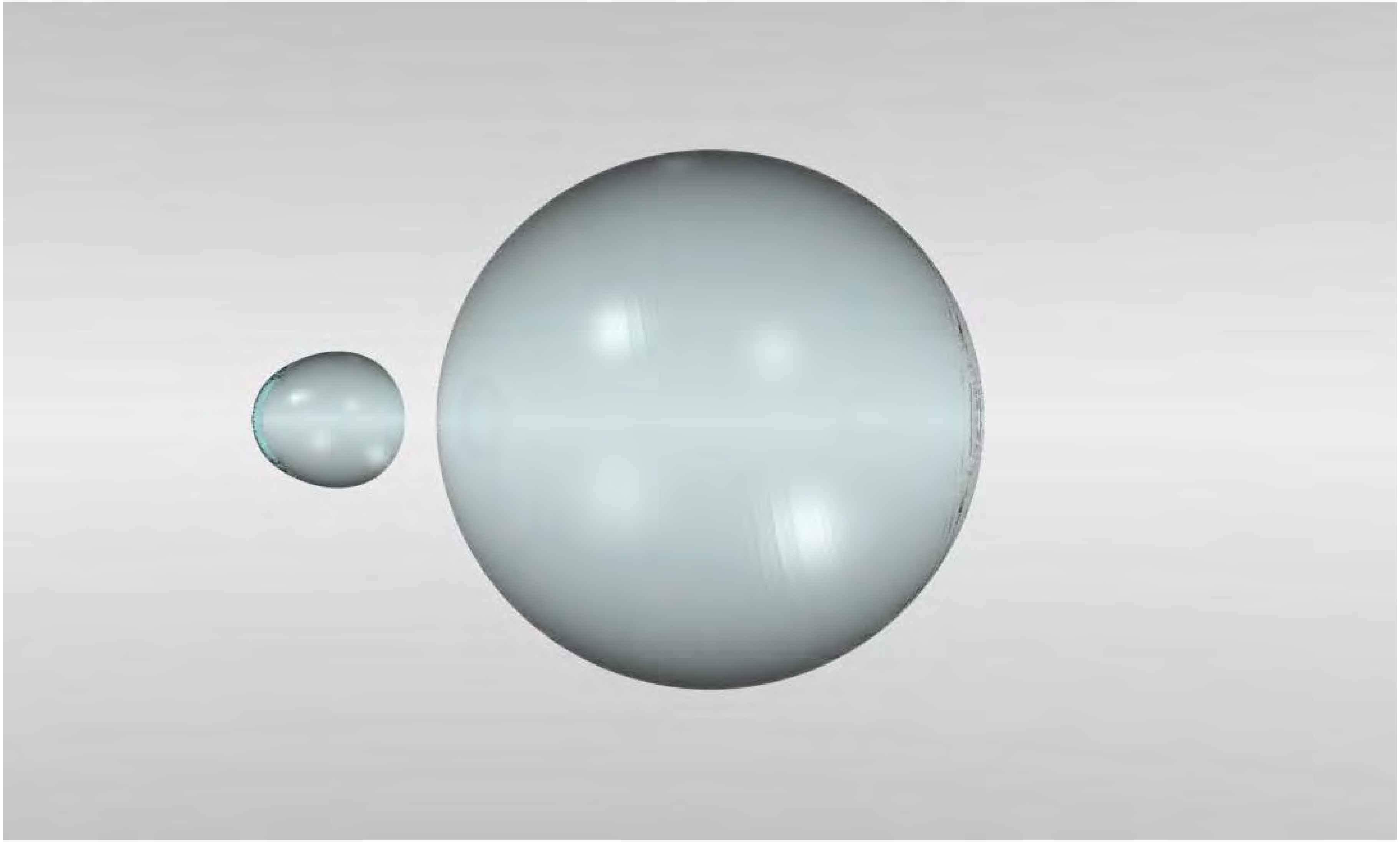
Droplet Diameter Ratio: 0.50



Conditions: water droplets in 1 atm. air, We=100, Re=1190.4, B=0, D_s=200 μm, U=6.0 m/s.

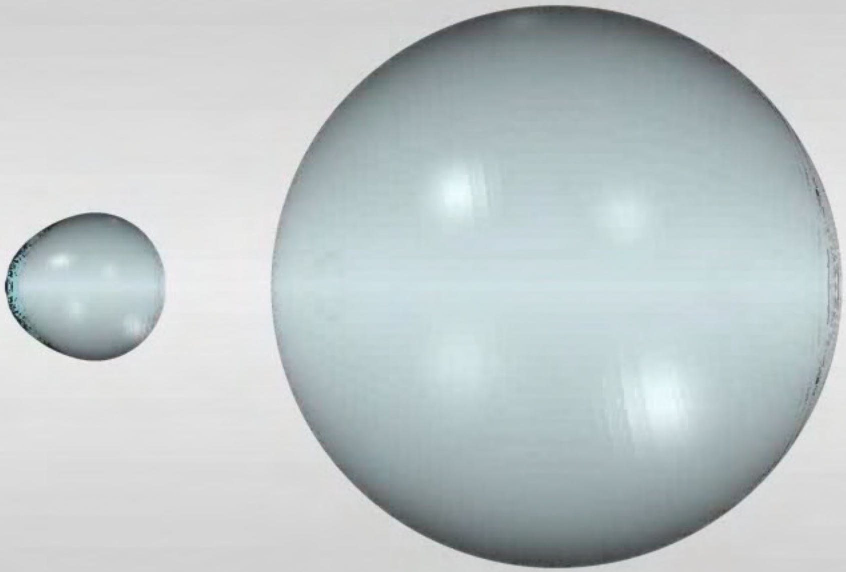
Unequal Merging (We = 100)

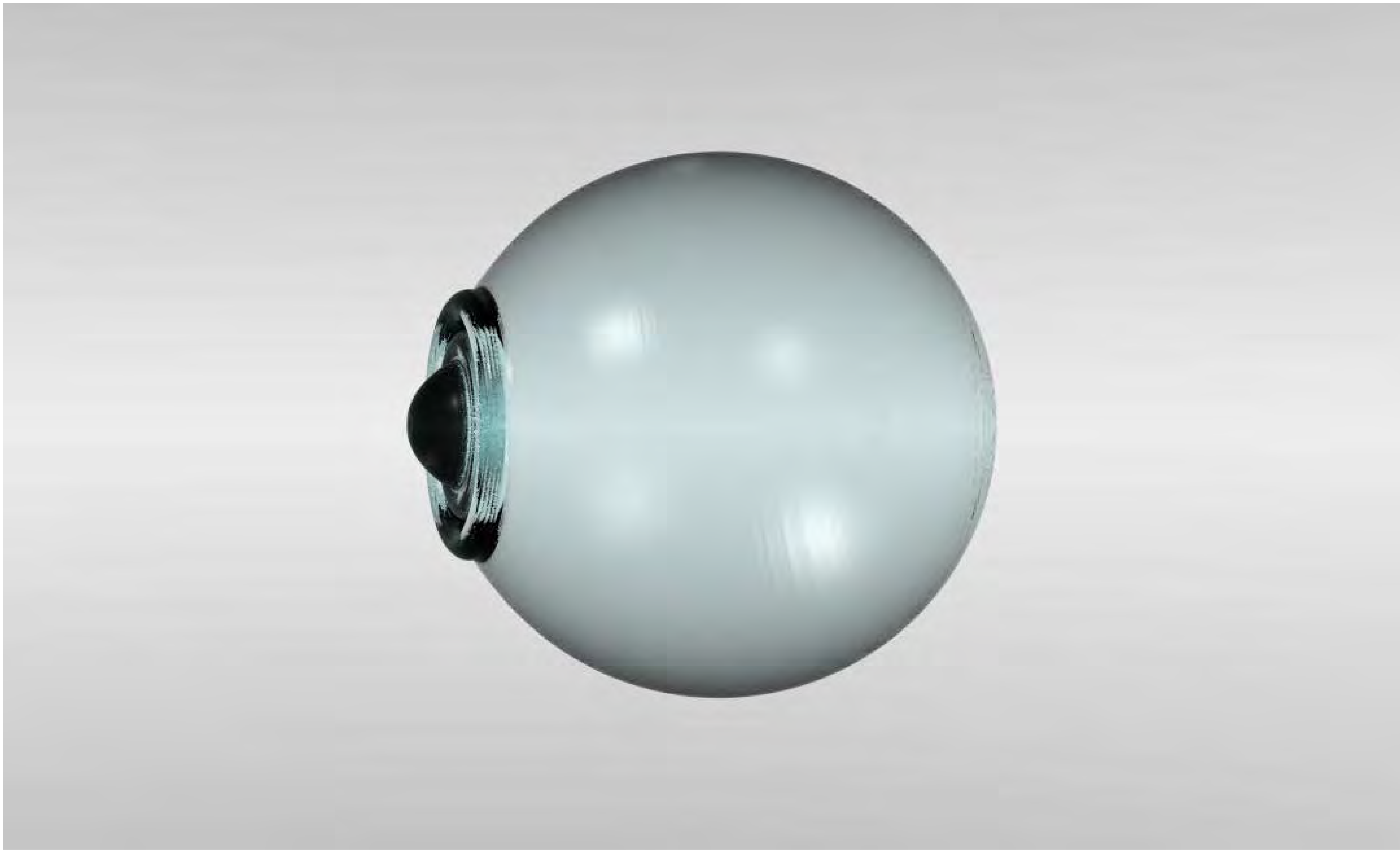
Droplet Diameter Ratio: 0.25

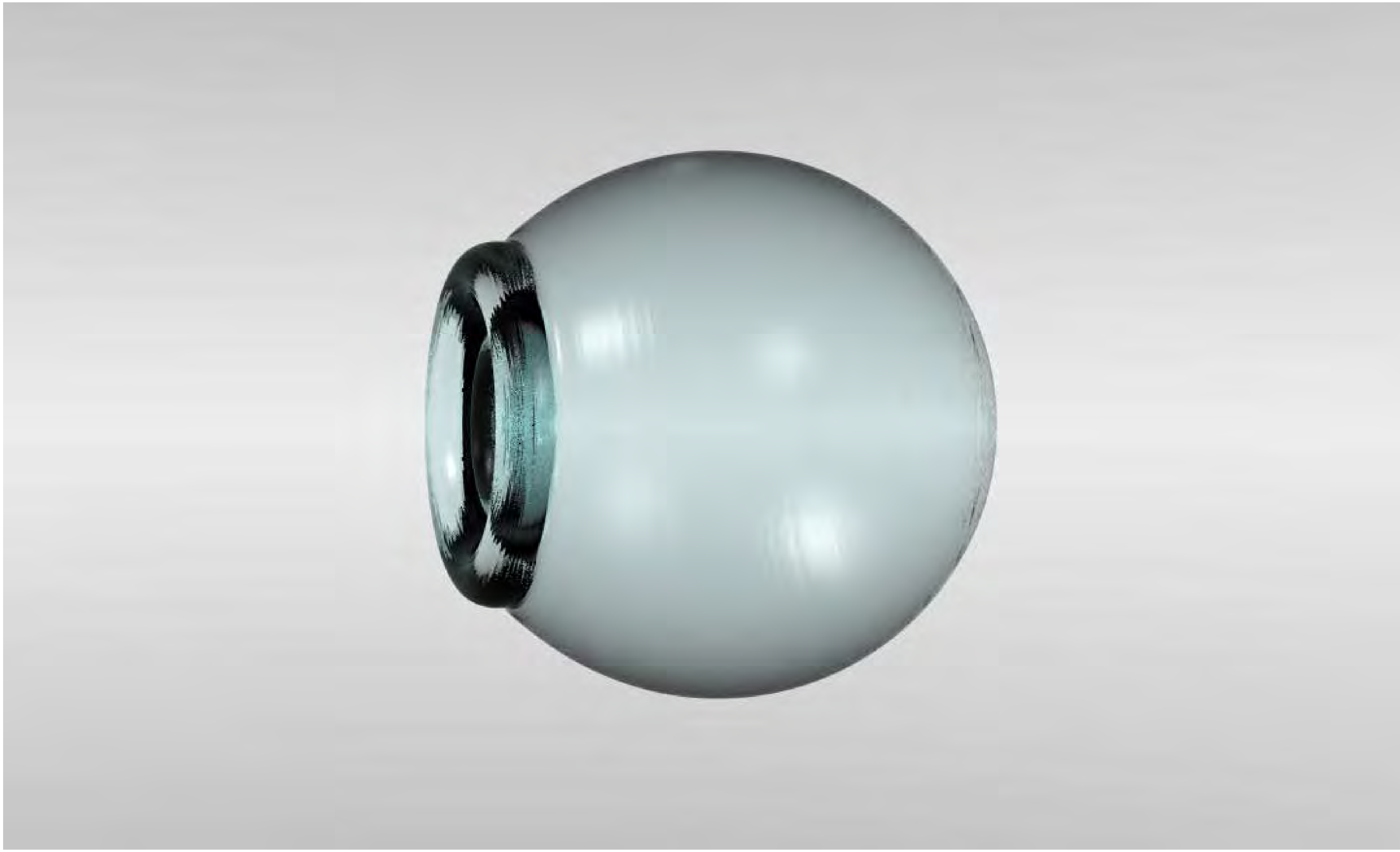


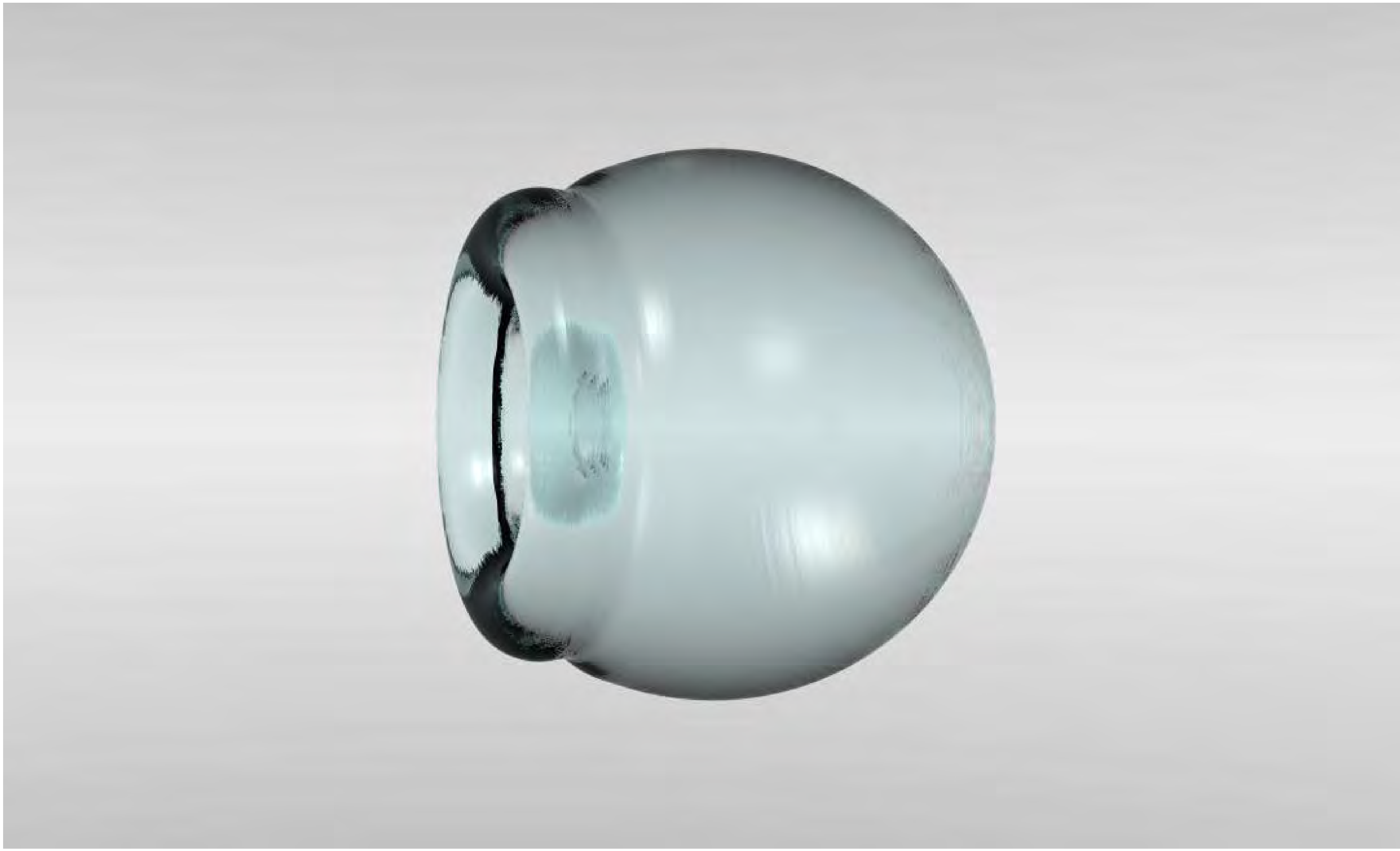
Conditions: water droplets in 1 atm. air, We=100, Re=851.9, B=0, Ds=100 μm, U=8.51 m/s.

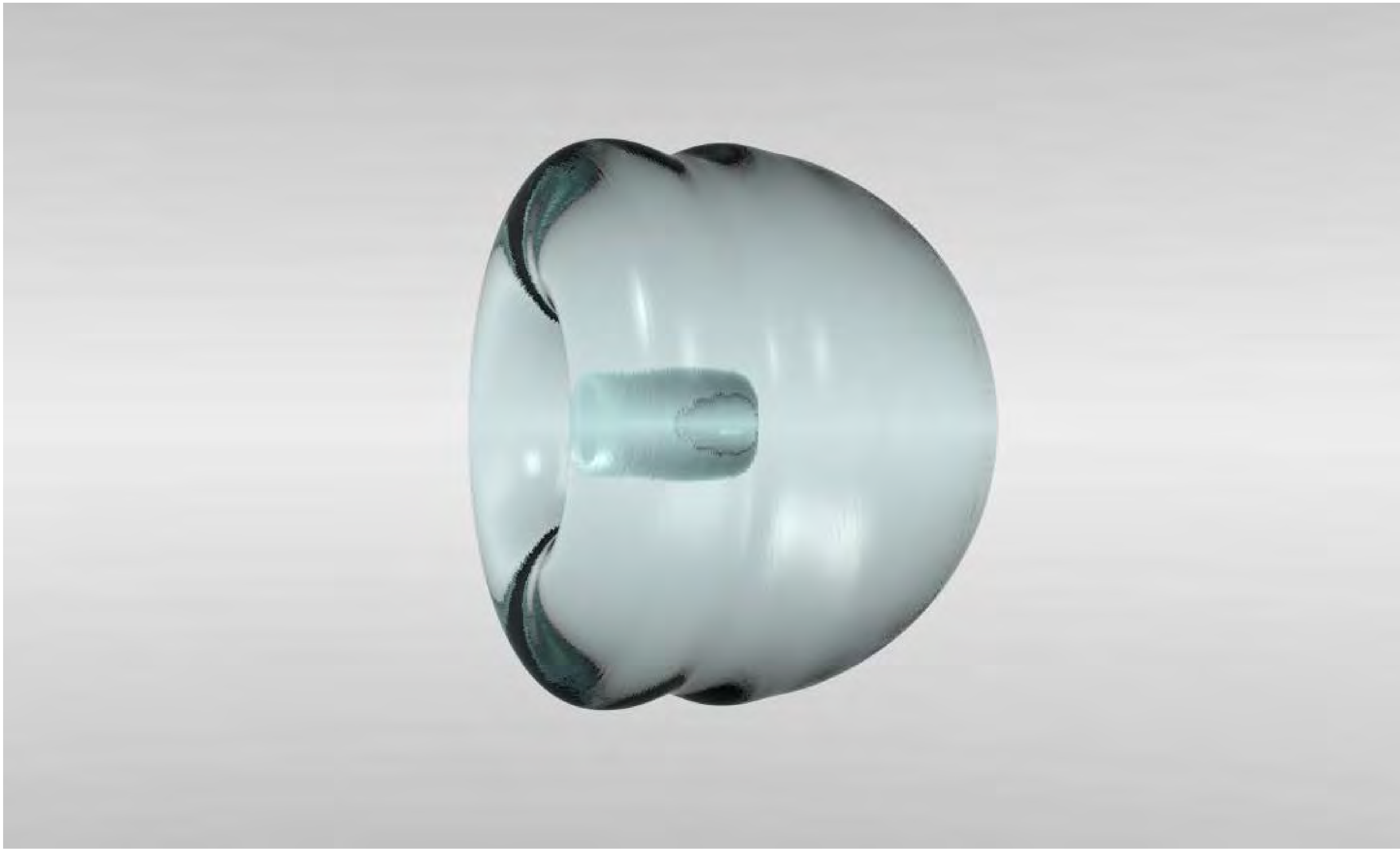
Movie

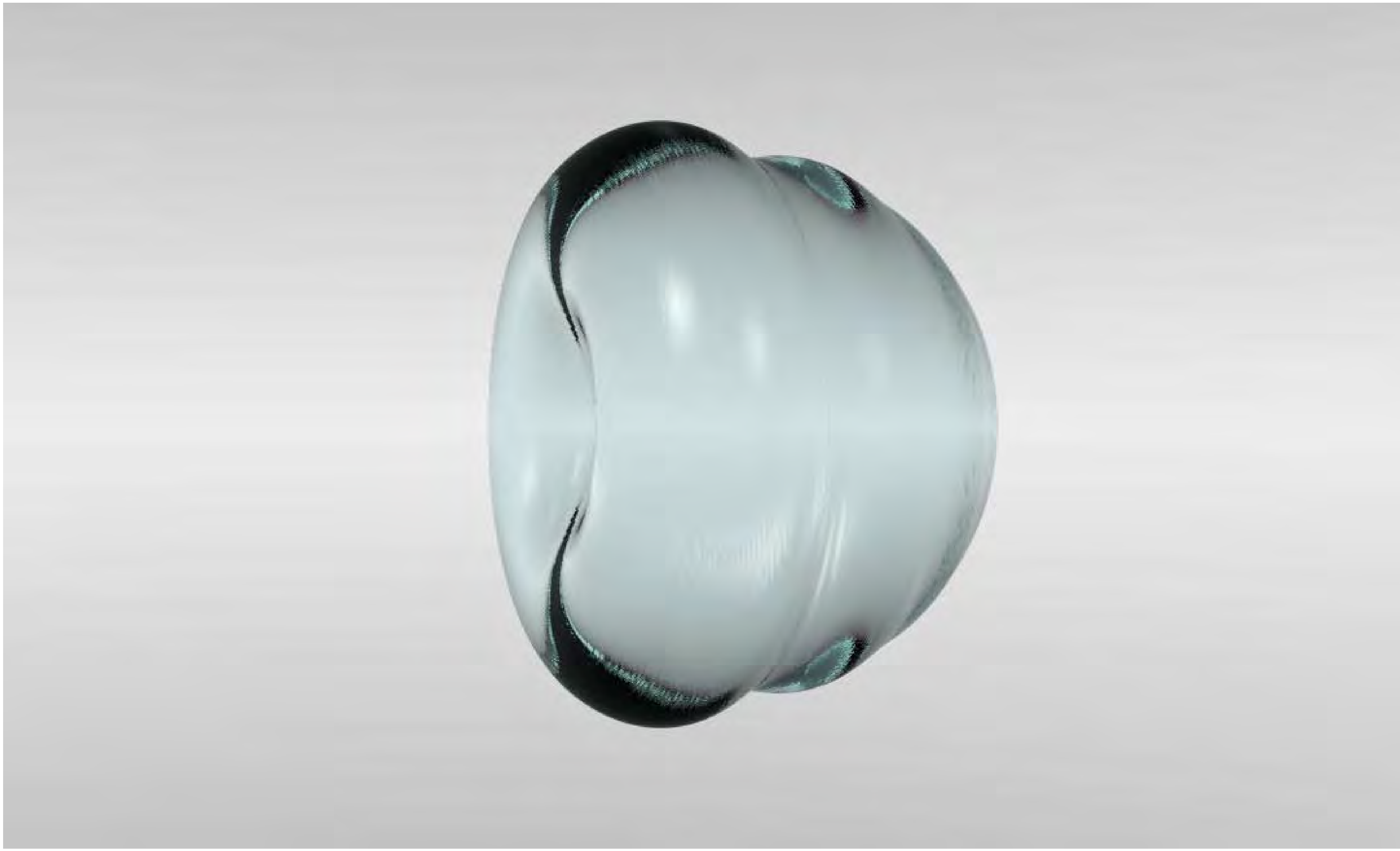


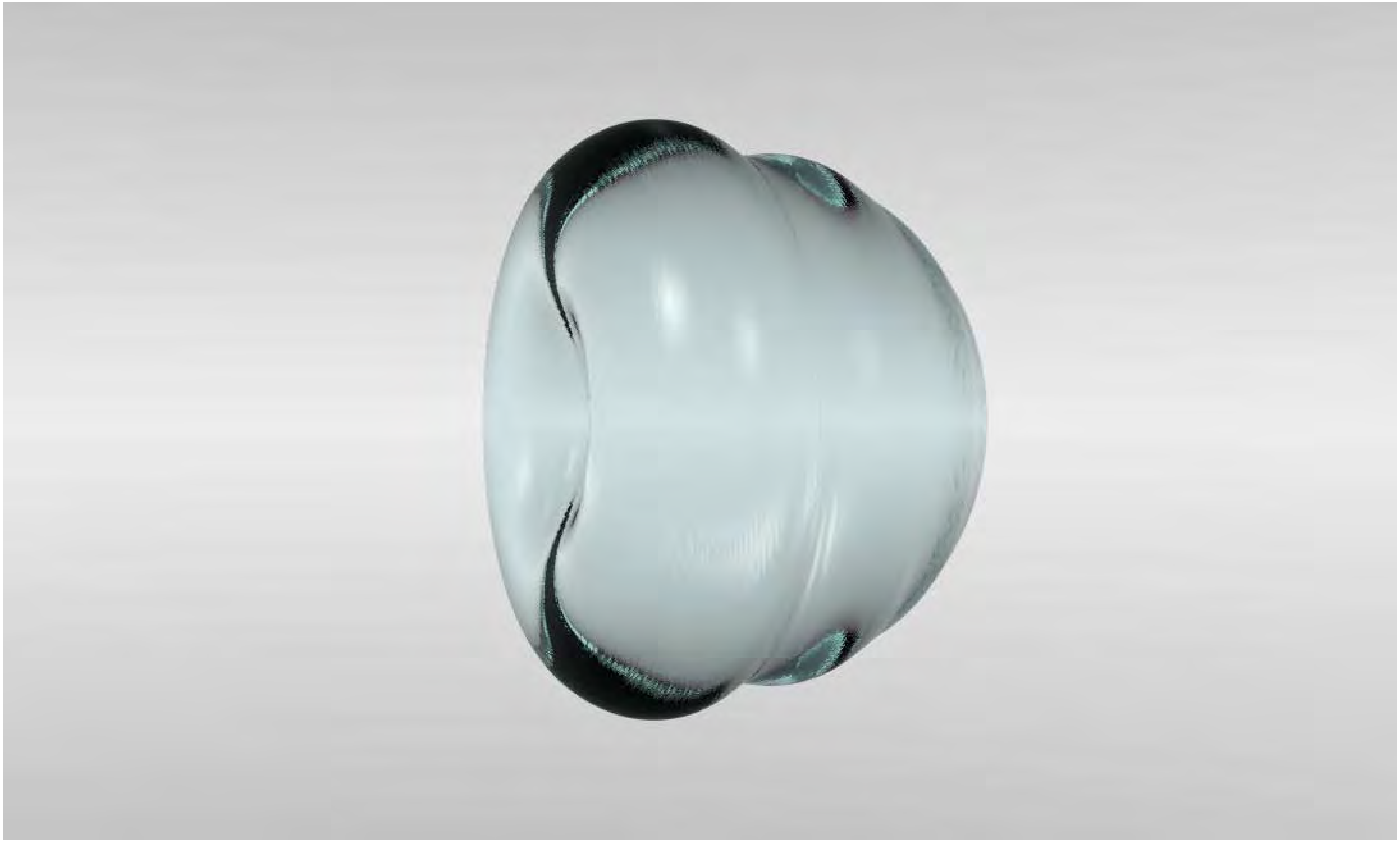


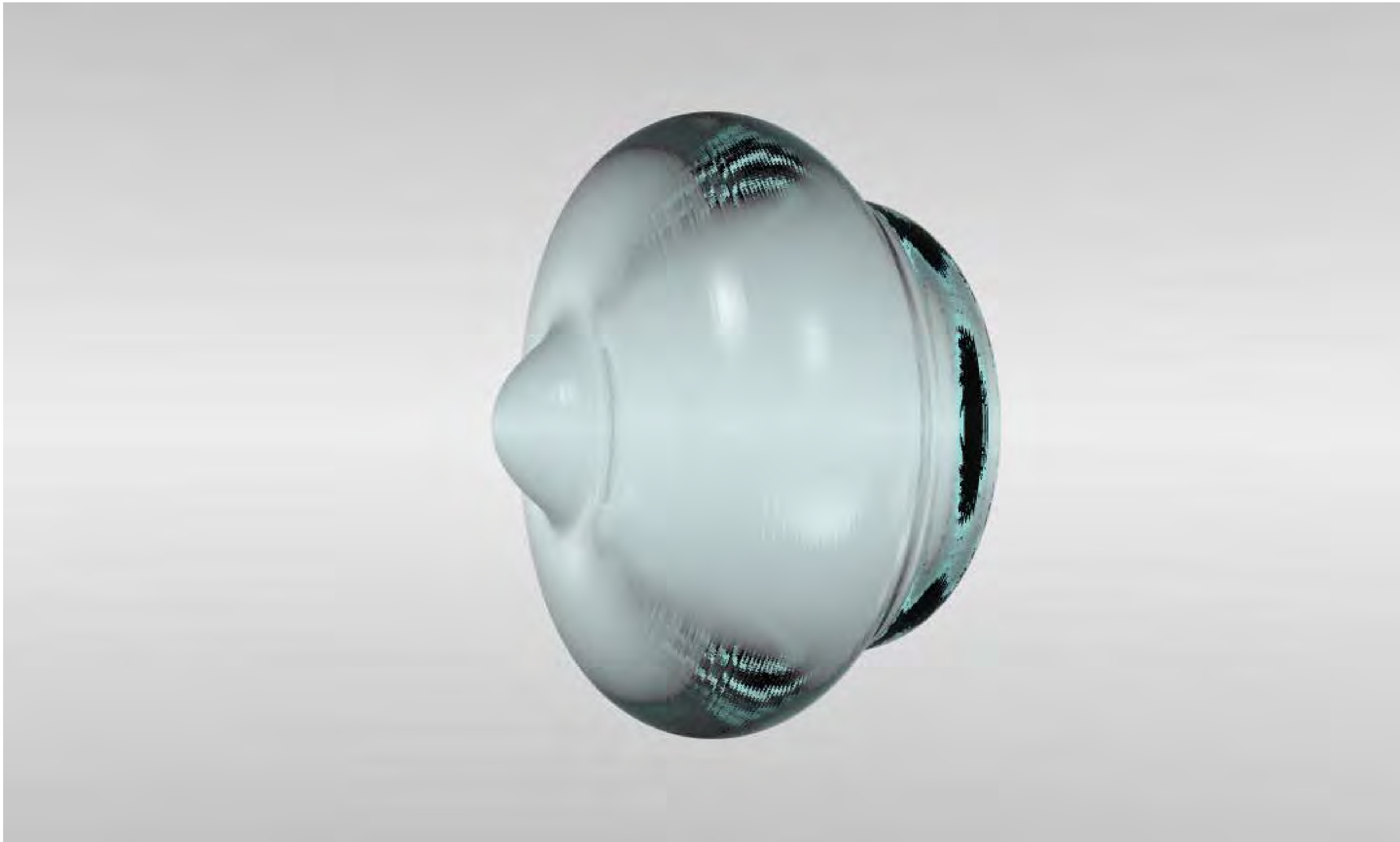






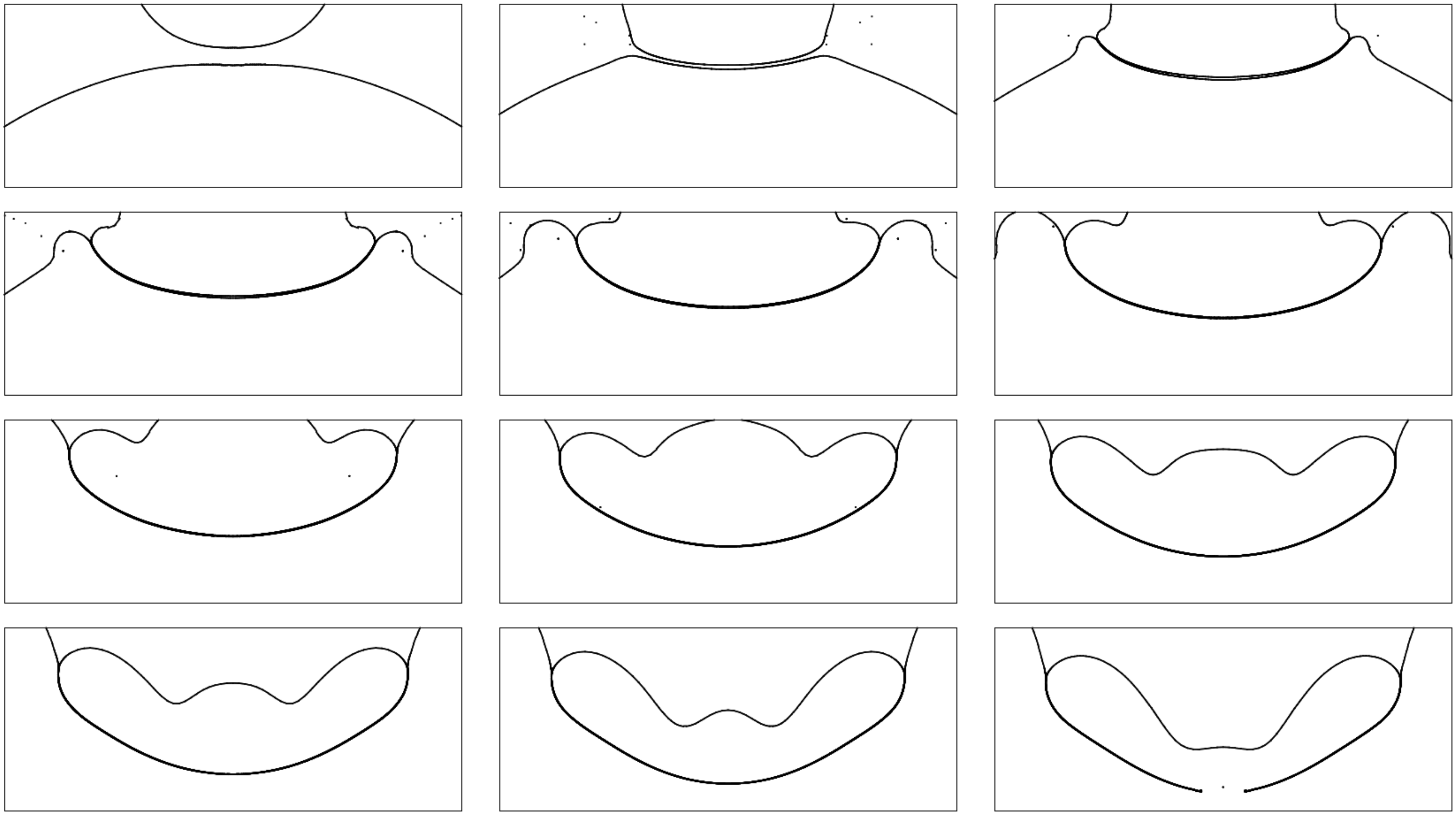






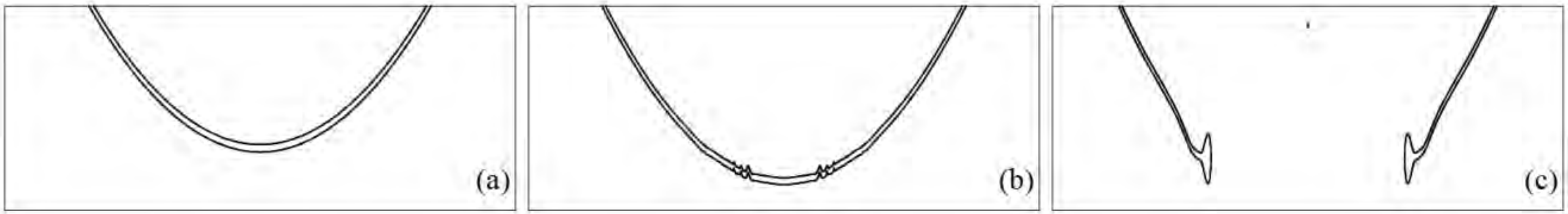
Unequal Merging (We = 100)

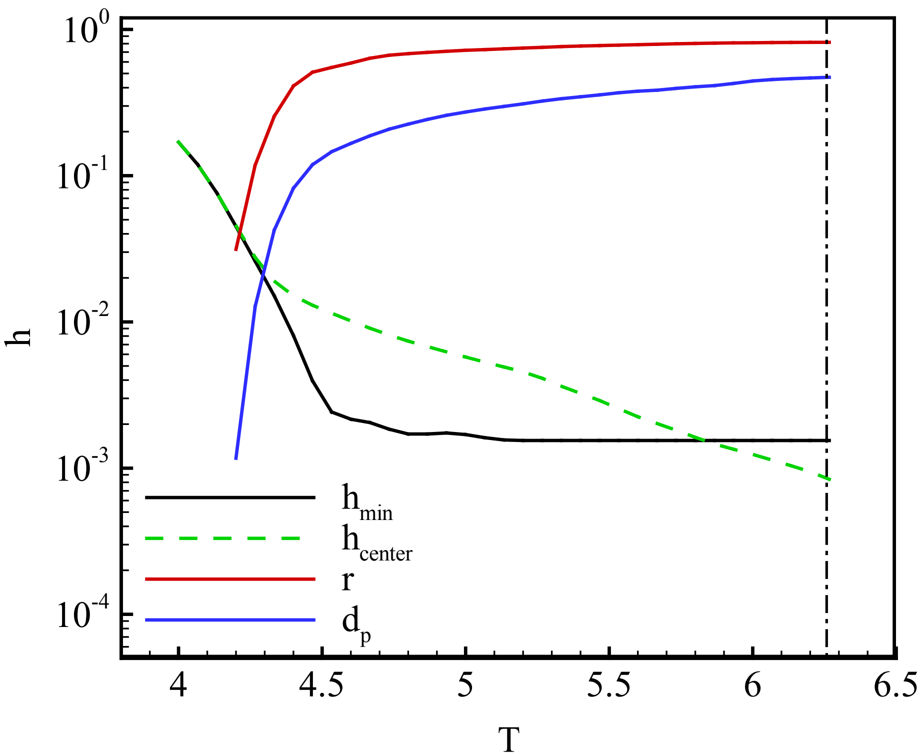
Droplet Diameter Ratio: 0.25



Conditions: water droplets in 1 atm. air, We=100, Re=851.9, B=0, Ds=100 µm, U=8.51 m/s.

Detail Deformation Before Rupture

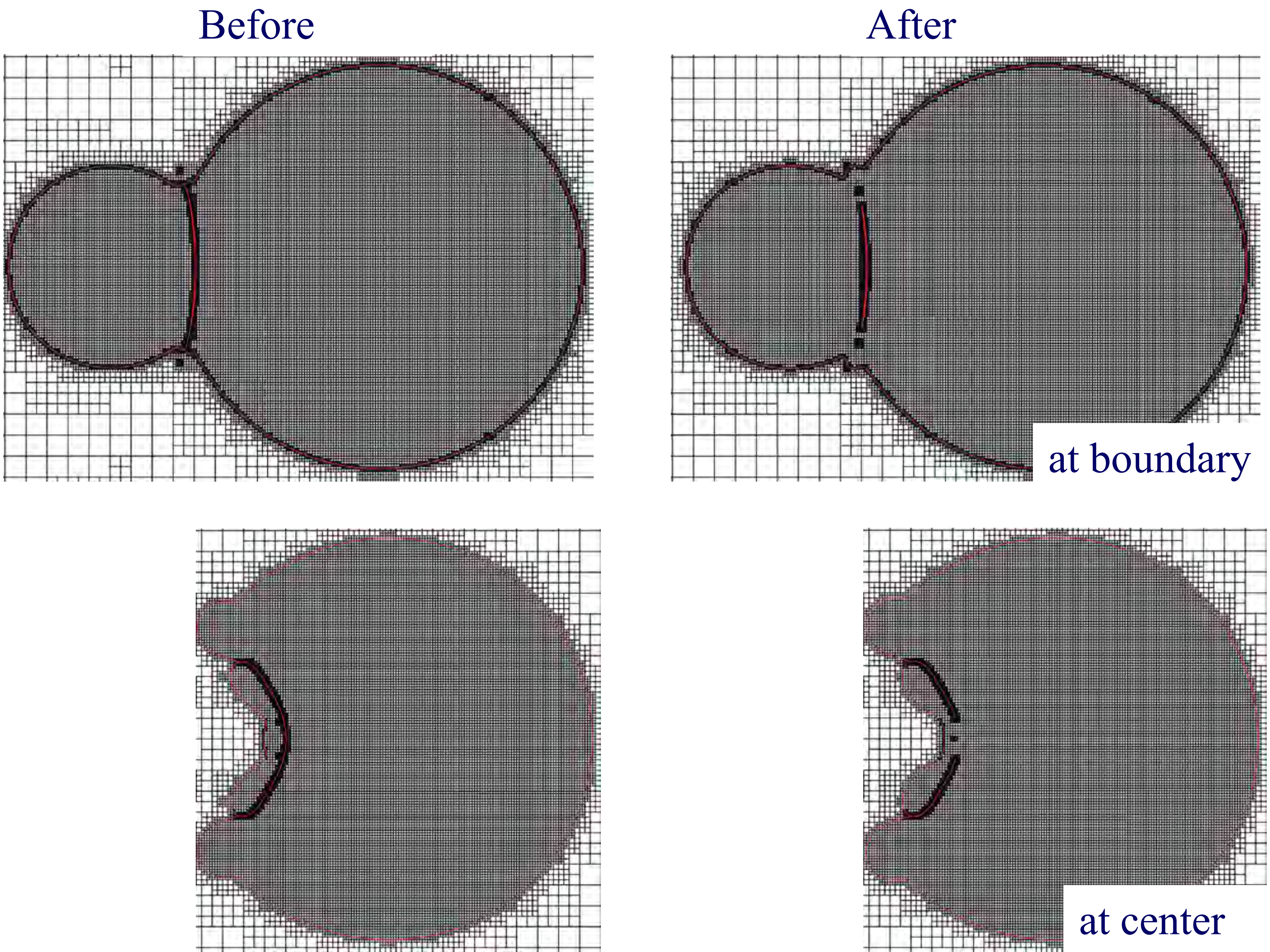




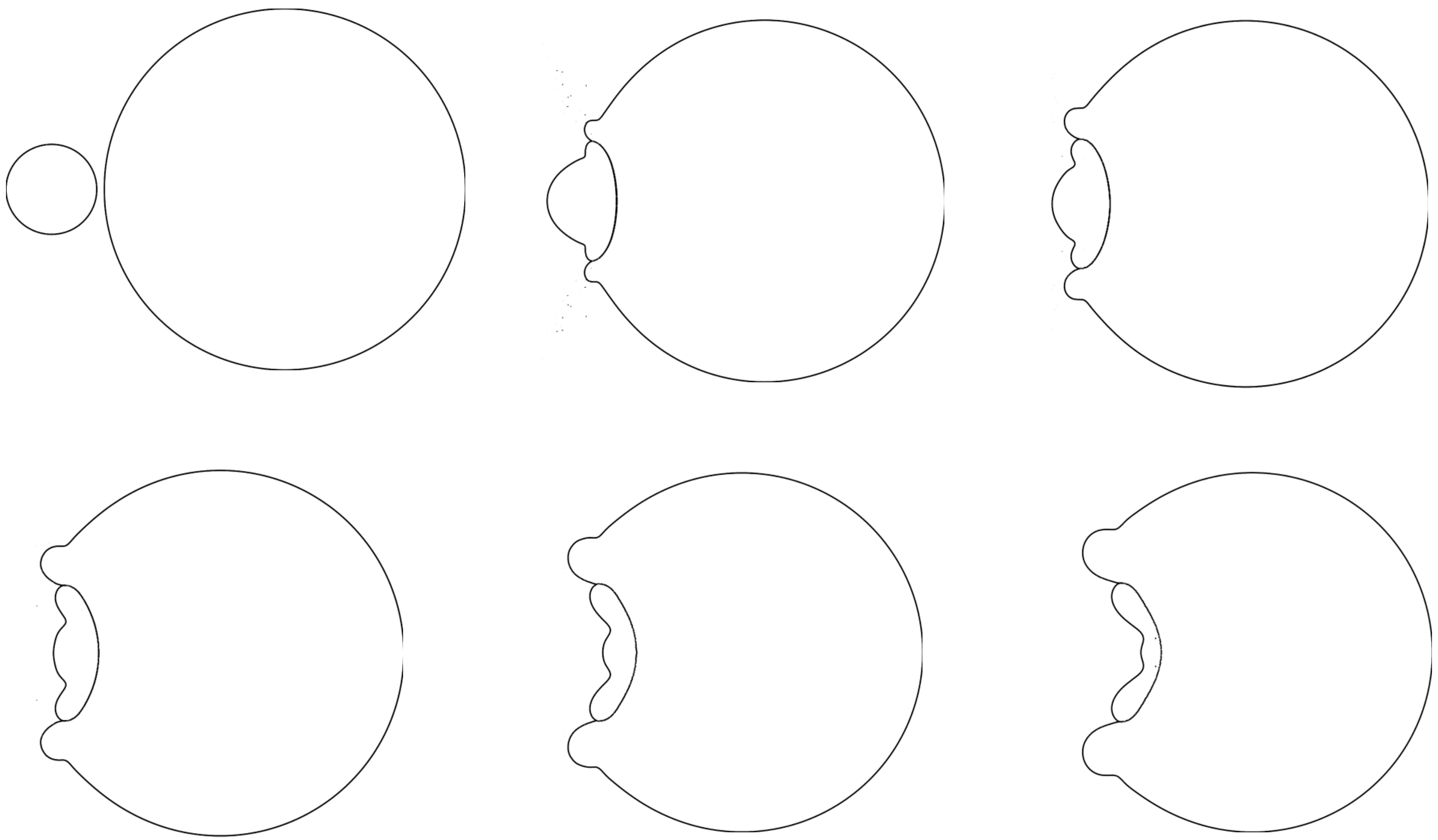
- After the formation of the gas film at T = 4.26, $\boldsymbol{h}_{min}$ decreases quickly and reaches a static stage with value of $1.55\times10^{-3}\boldsymbol{D}$, while $\boldsymbol{h}_{center}$ shows a continually decreasing.
- The minimum value of $\boldsymbol{h}_{center}$ is reached at merging point with a value of $8.39\times10^{-4}\boldsymbol{D}$ which is smaller than $\boldsymbol{h}_{min}$.
- This means a continually compress between the two droplets.

Conditions: water droplets in 1 atm. air, We=100, Re=851.9, B=0, Ds=100 µm, U=8.51 m/s.

Ruptures of Thin Gas Films (We = 100)



Detail Deformation Before Rupture



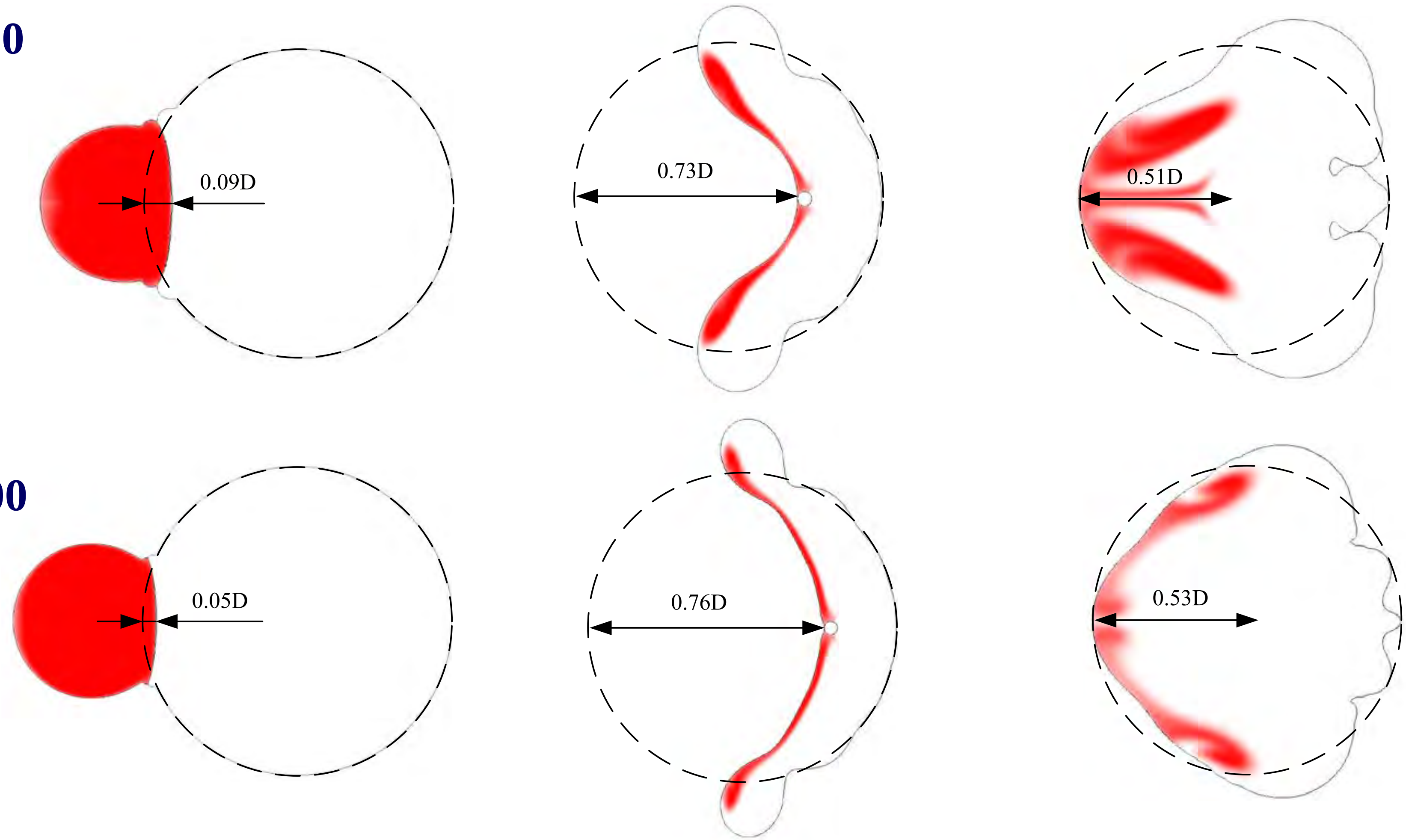
Conditions: water droplets in 1 atm. air, We=100, Re=851.9, B=0, Ds=100 μm, U=2.69 m/s.

Liquid Phase Mixing

Droplet Diameter Ratio: 0.50

We = 50

We = 100



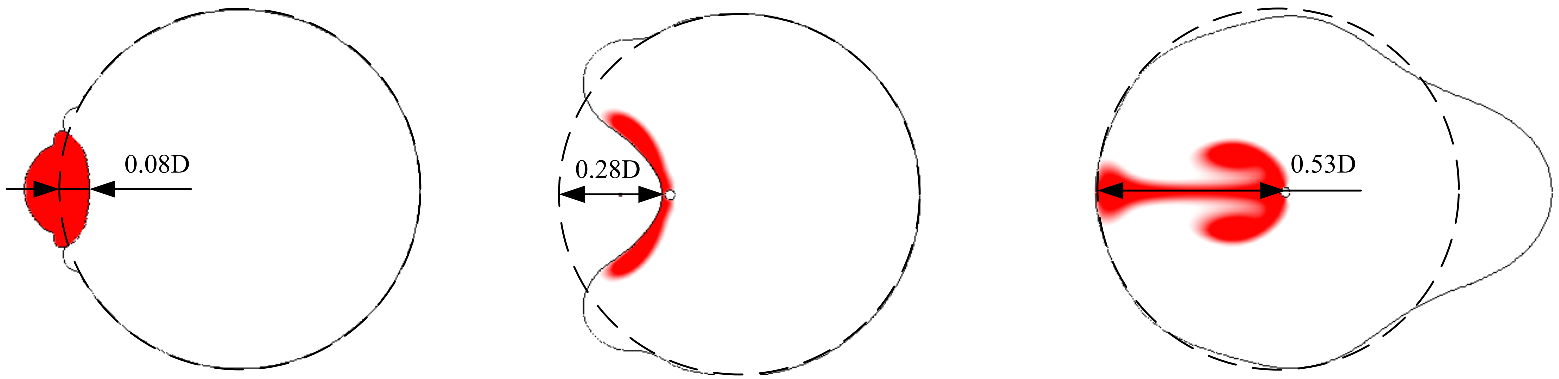
Georgia Tech

Liquid Phase Mixing

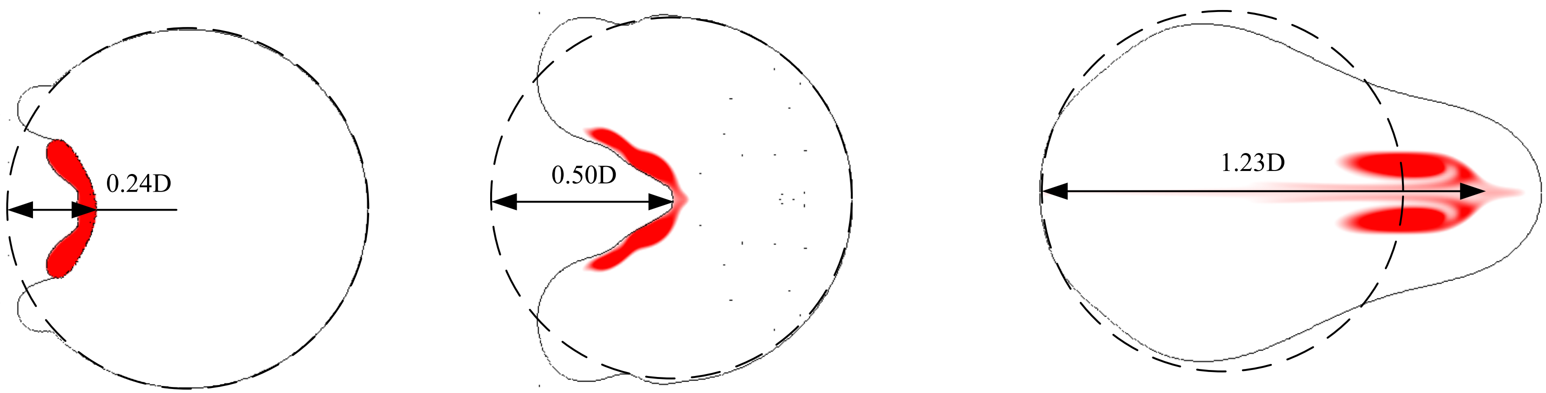
Droplet Diameter Ratio: 0.25

School of Aerospace Engineering

We = 50



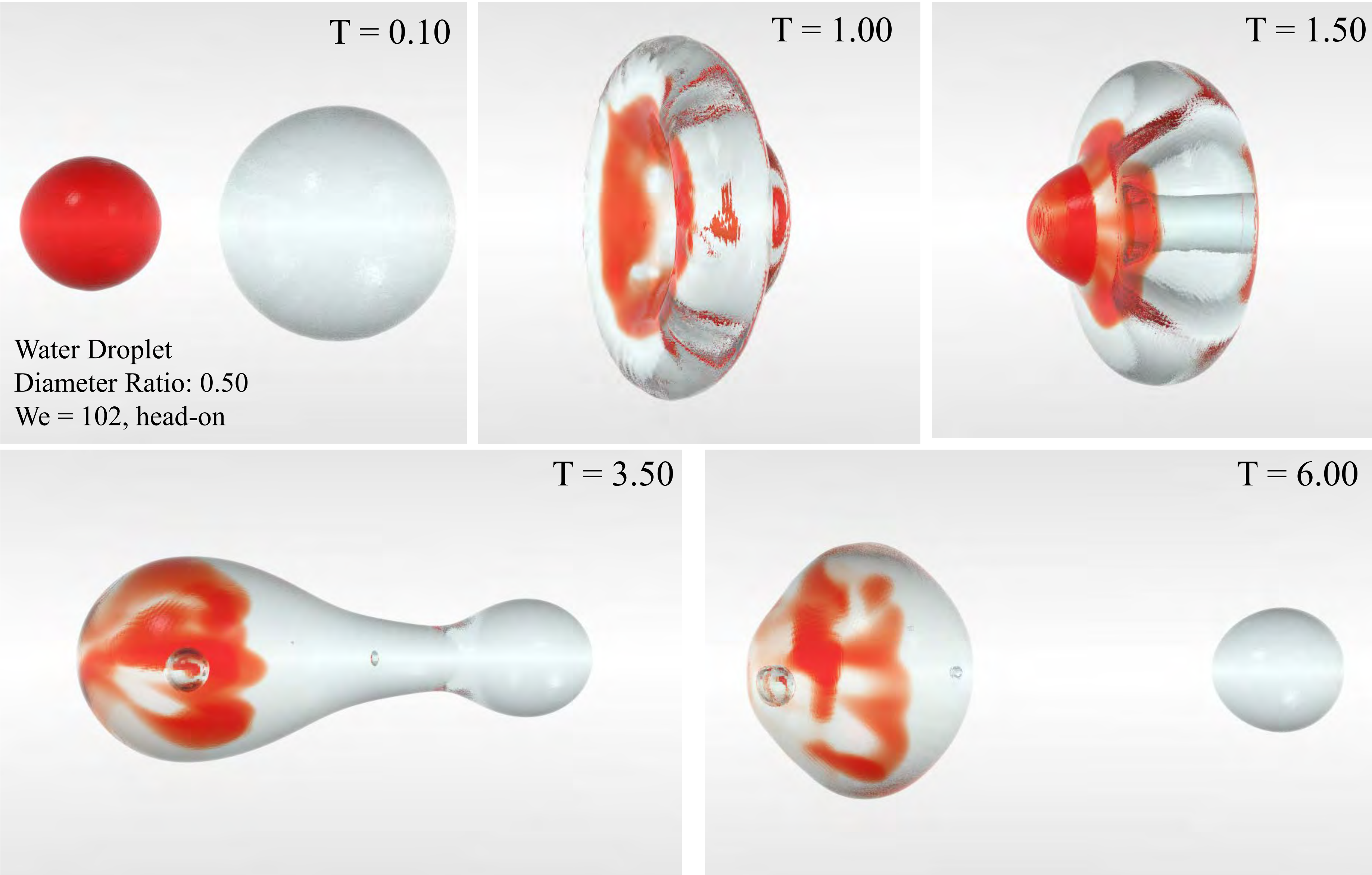
We = 100



Georgia Tech

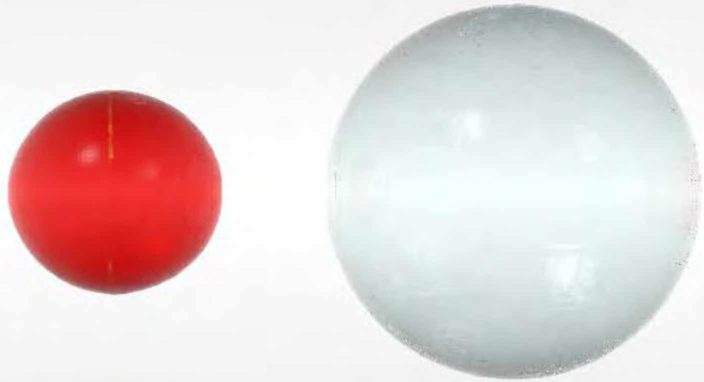
Unequal Reflexive Separation

School of Aerospace Engineering

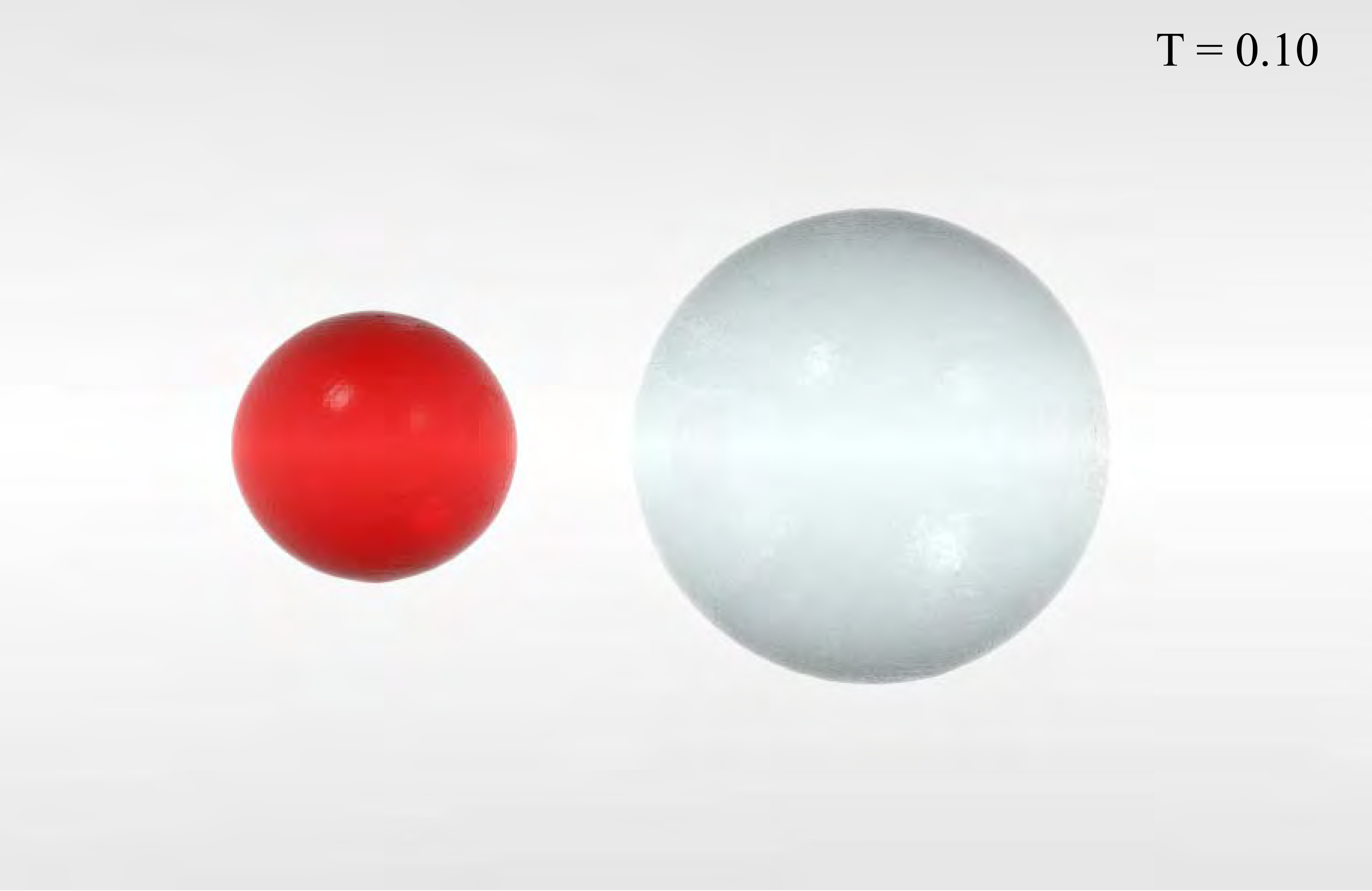


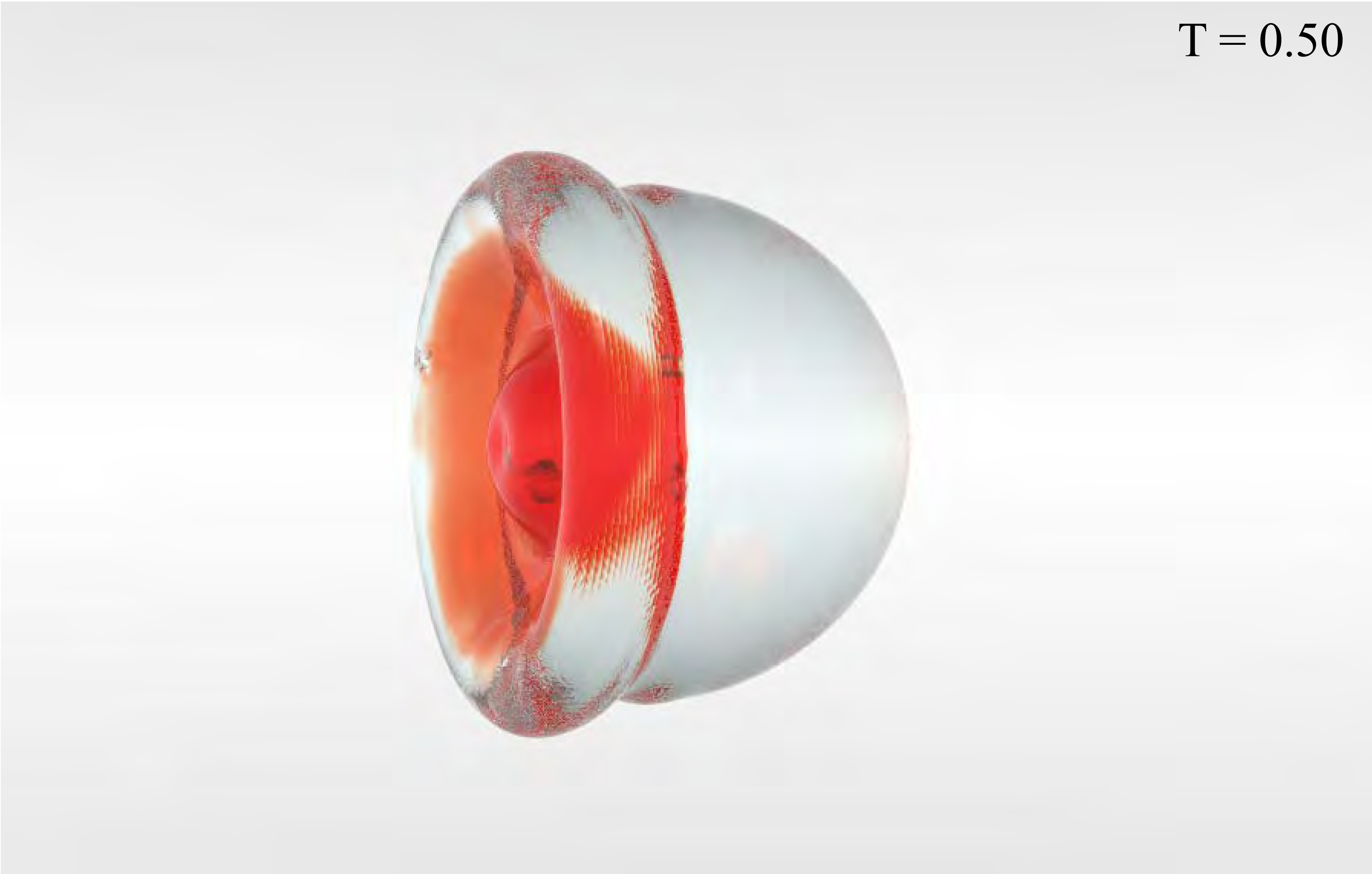
Unequal Reflexive Separation

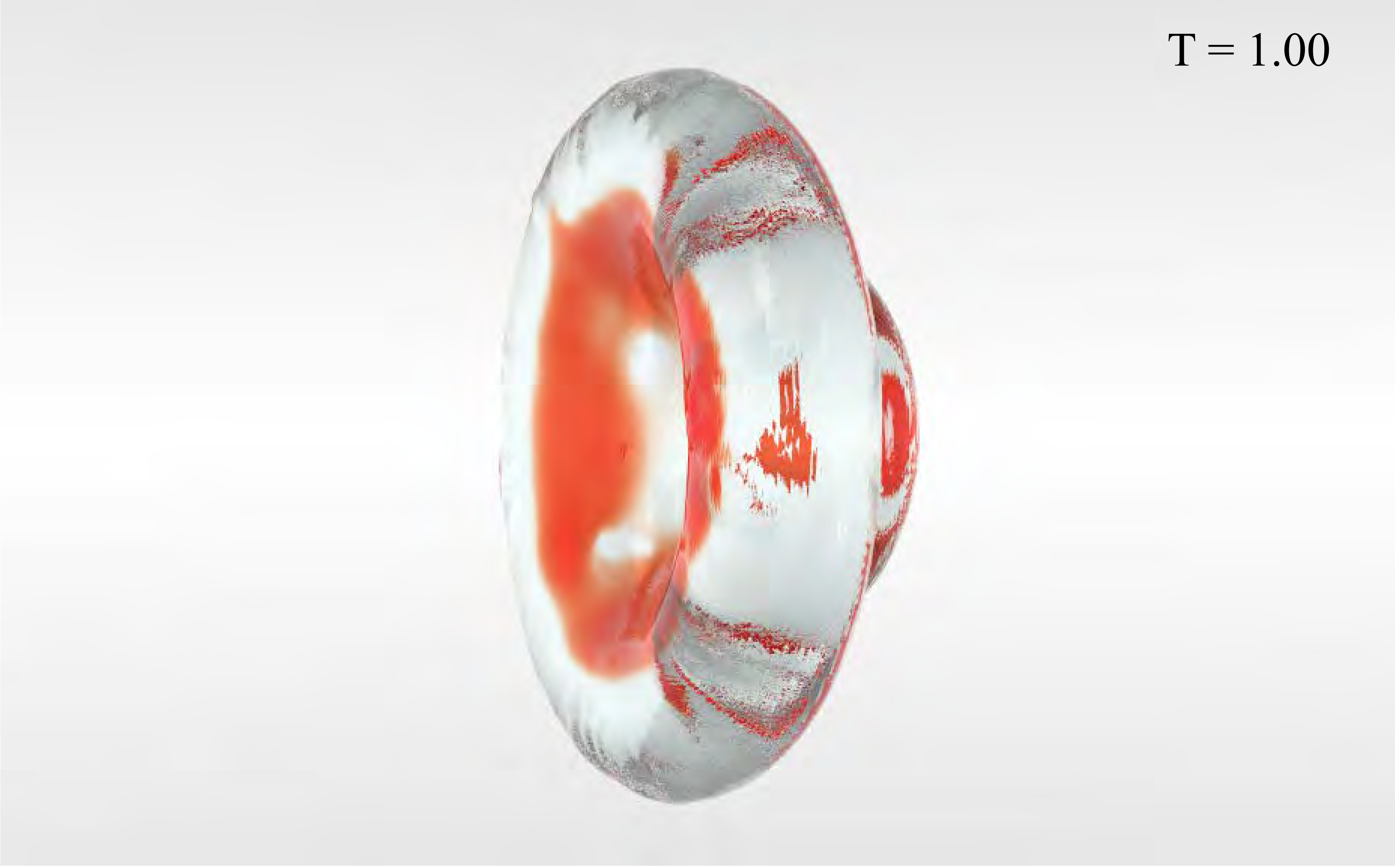
Movie

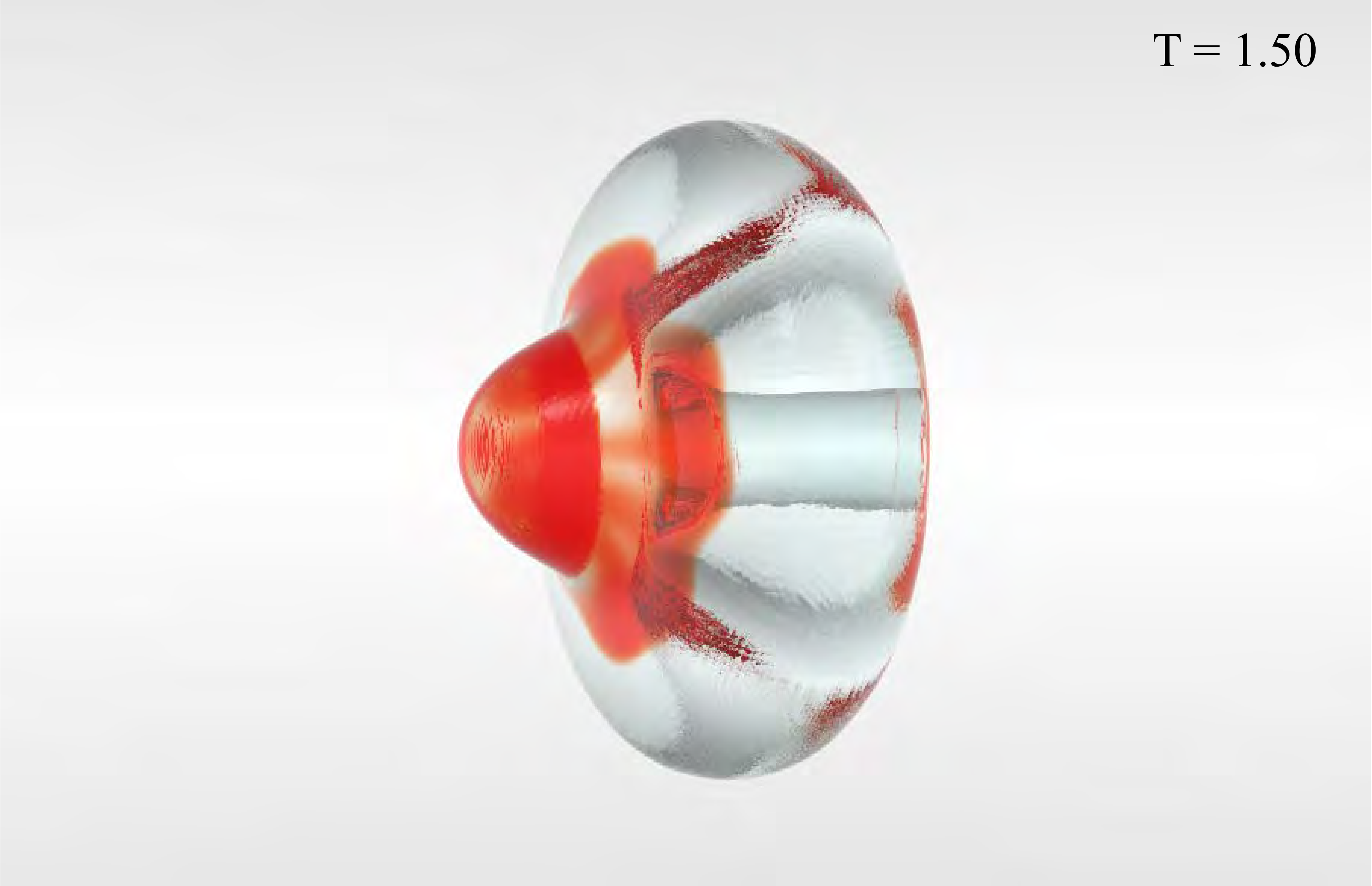


Diameter Ratio: 0.50




T = 0.50

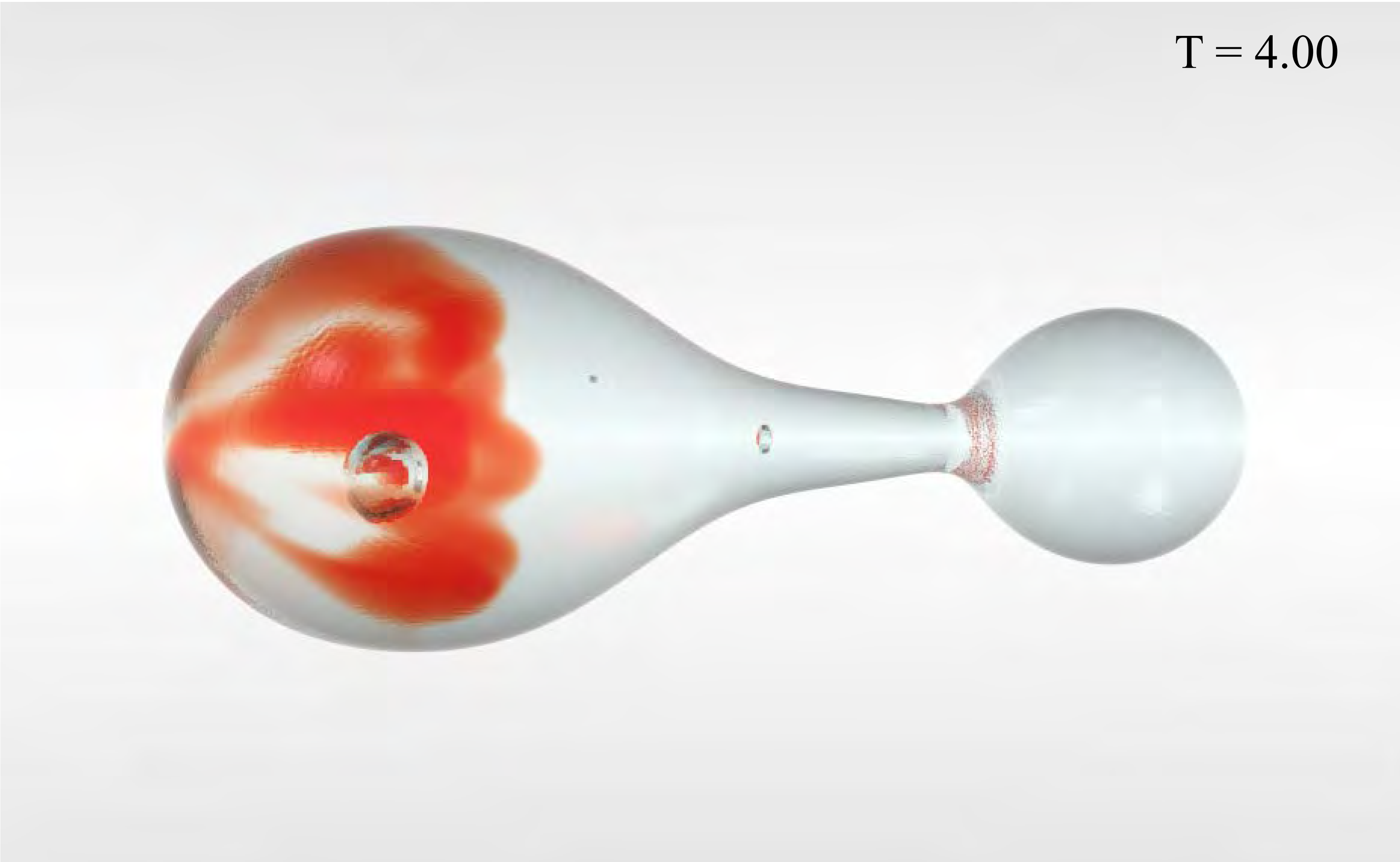

T = 1.00

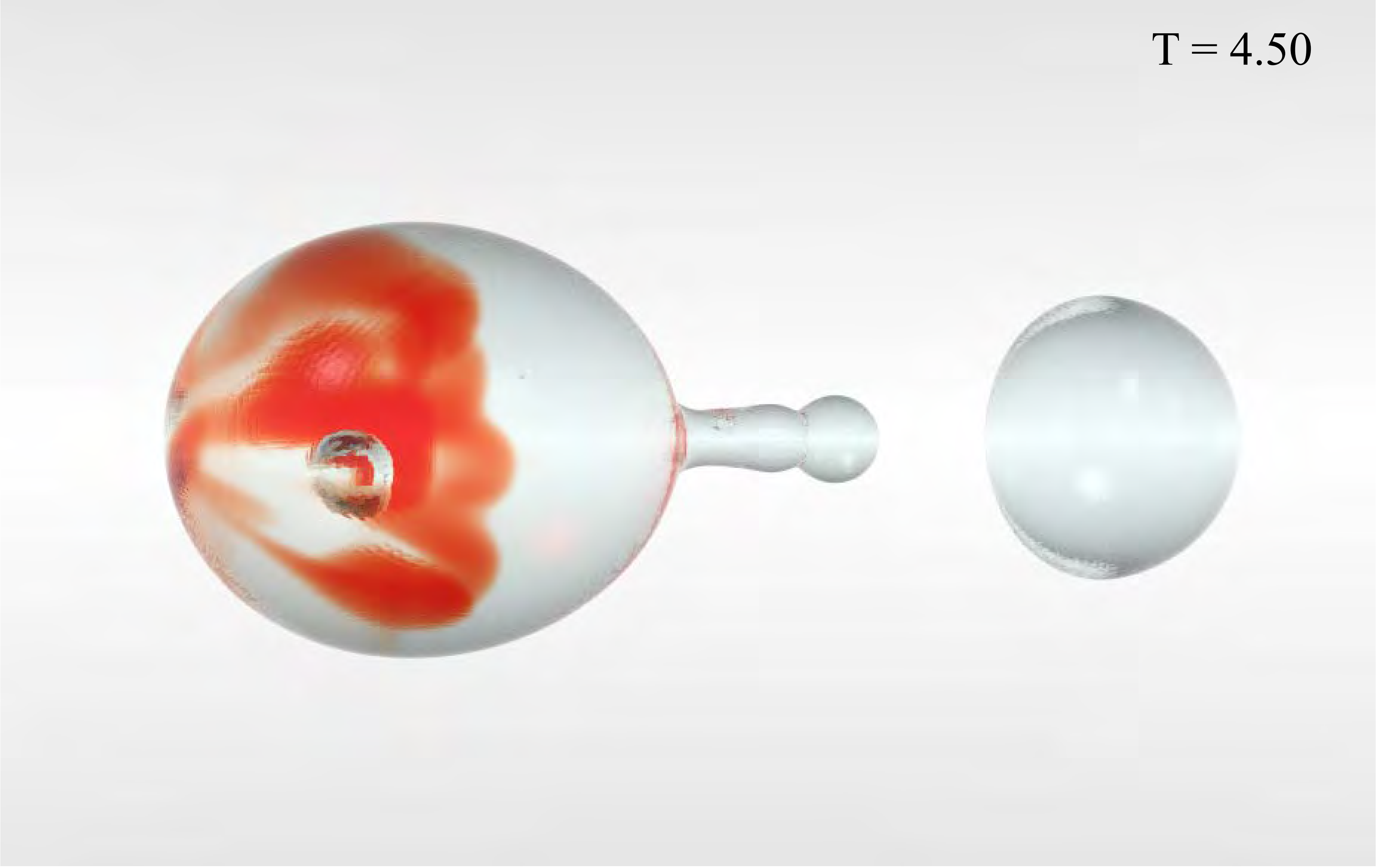

T = 1.50

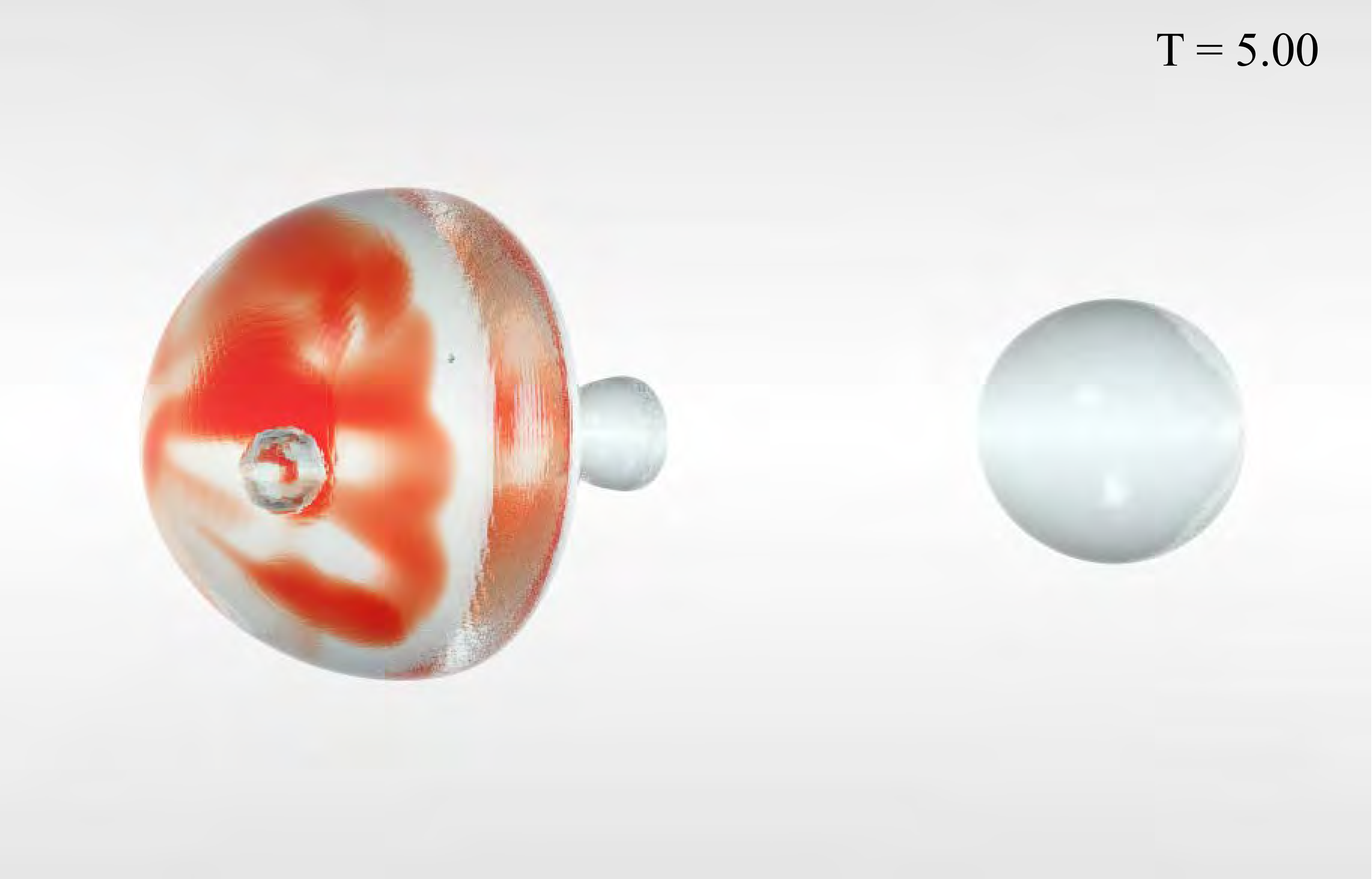

T = 2.50

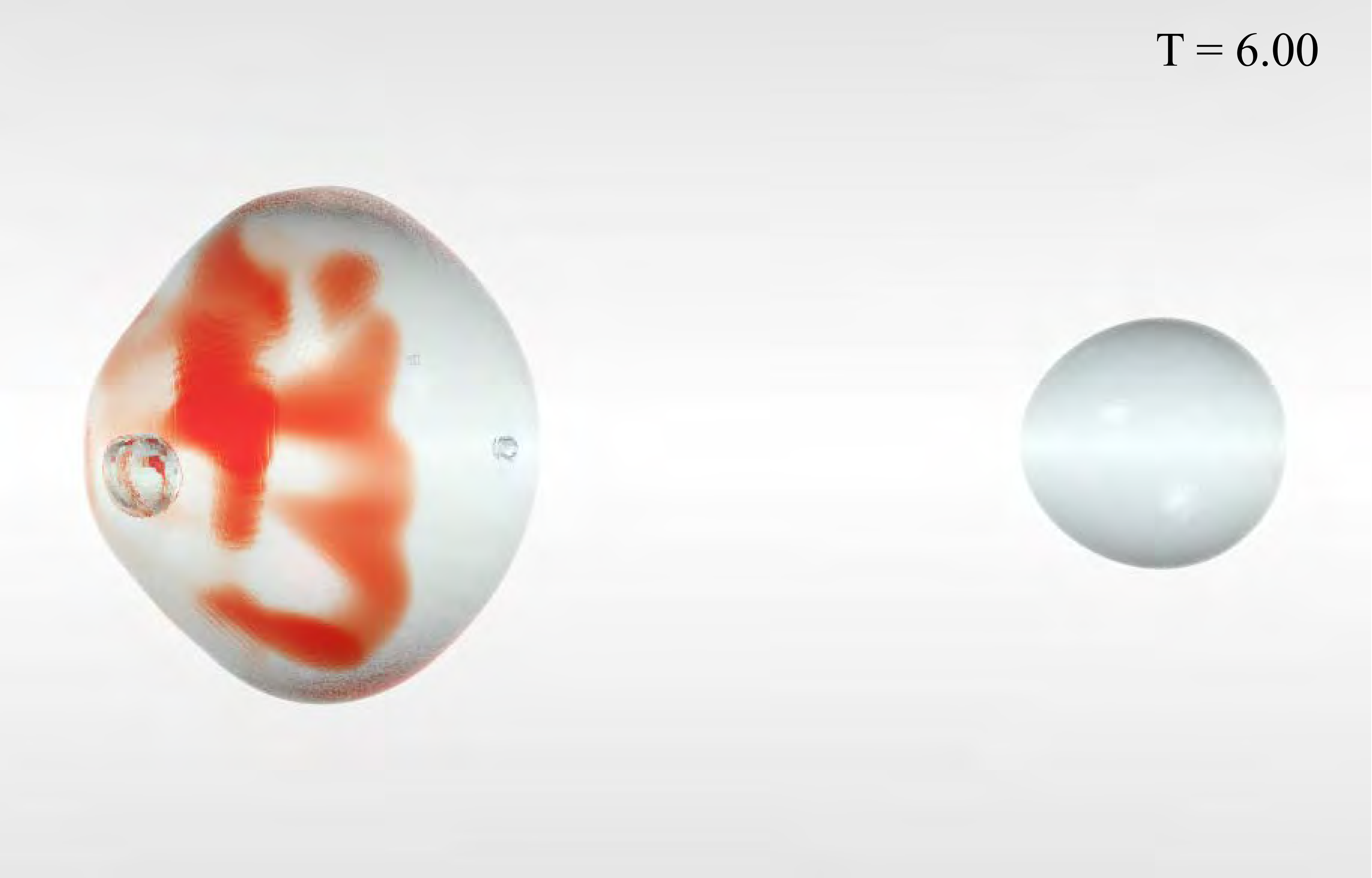

T = 3.00


T = 3.50

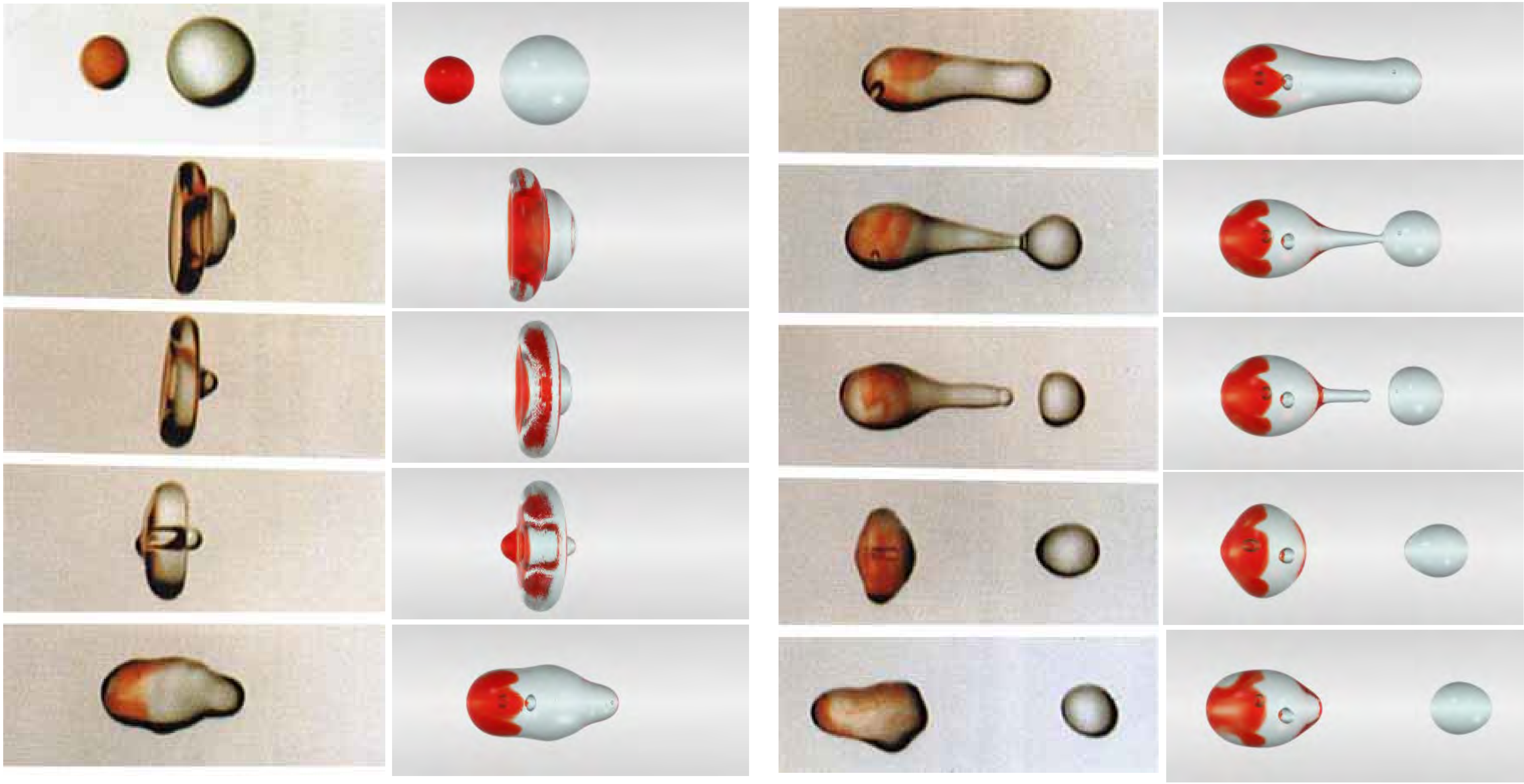

T = 4.00


T = 4.50


T = 5.00


T = 6.00

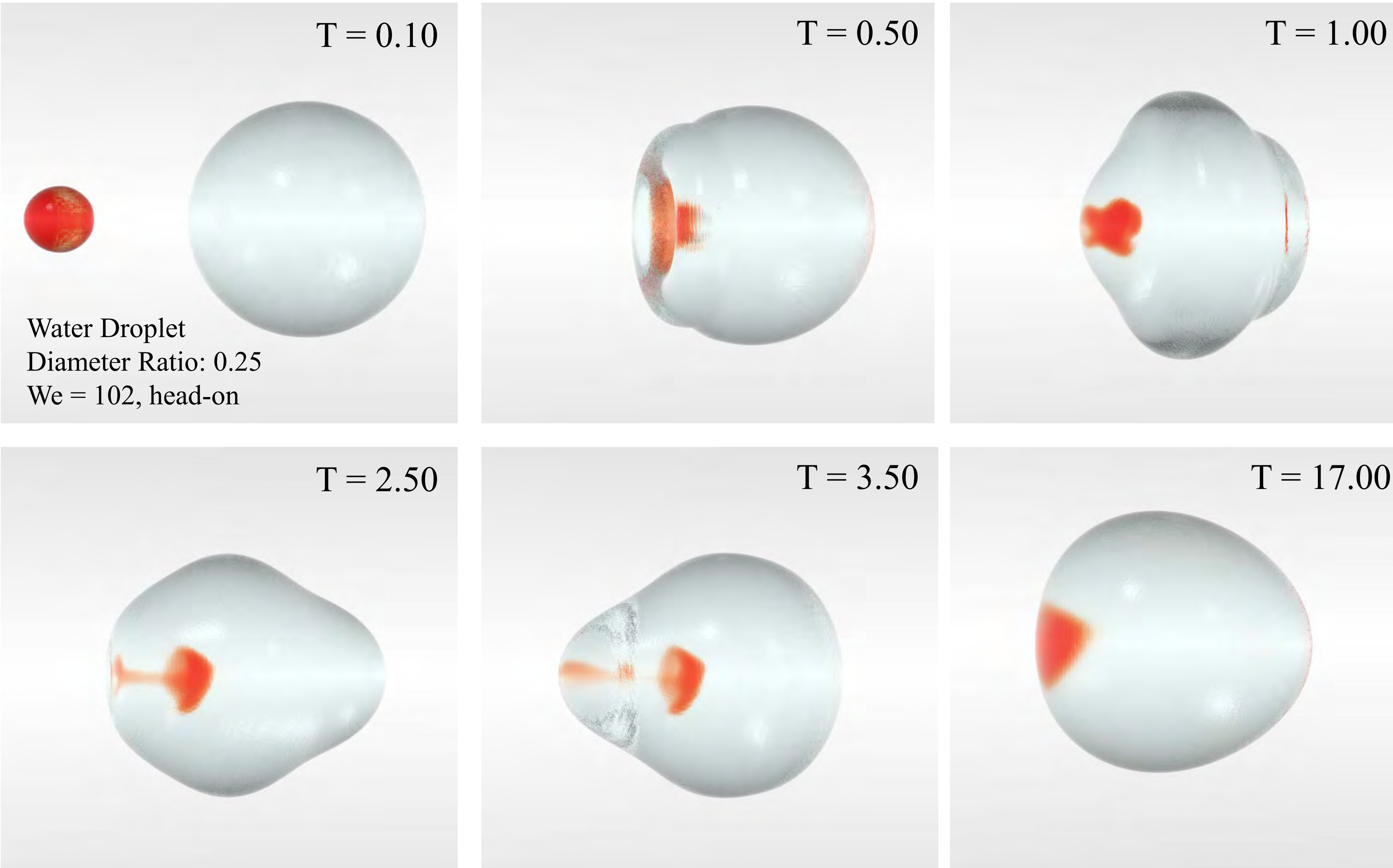
Comparison with Experimental Images



Ref: Coalescence and separation in binary collisions of liquid drops, JFM 1990

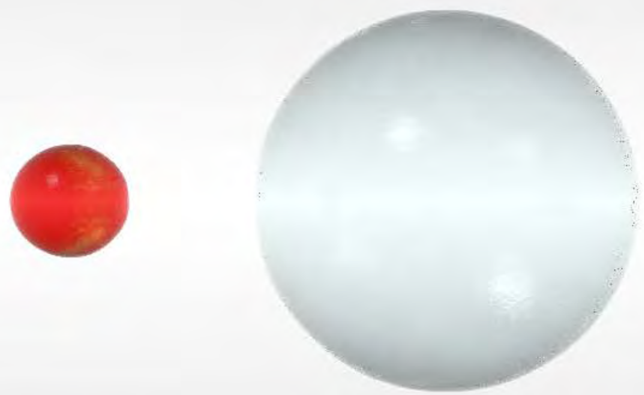
Unequal Coalescence Collision

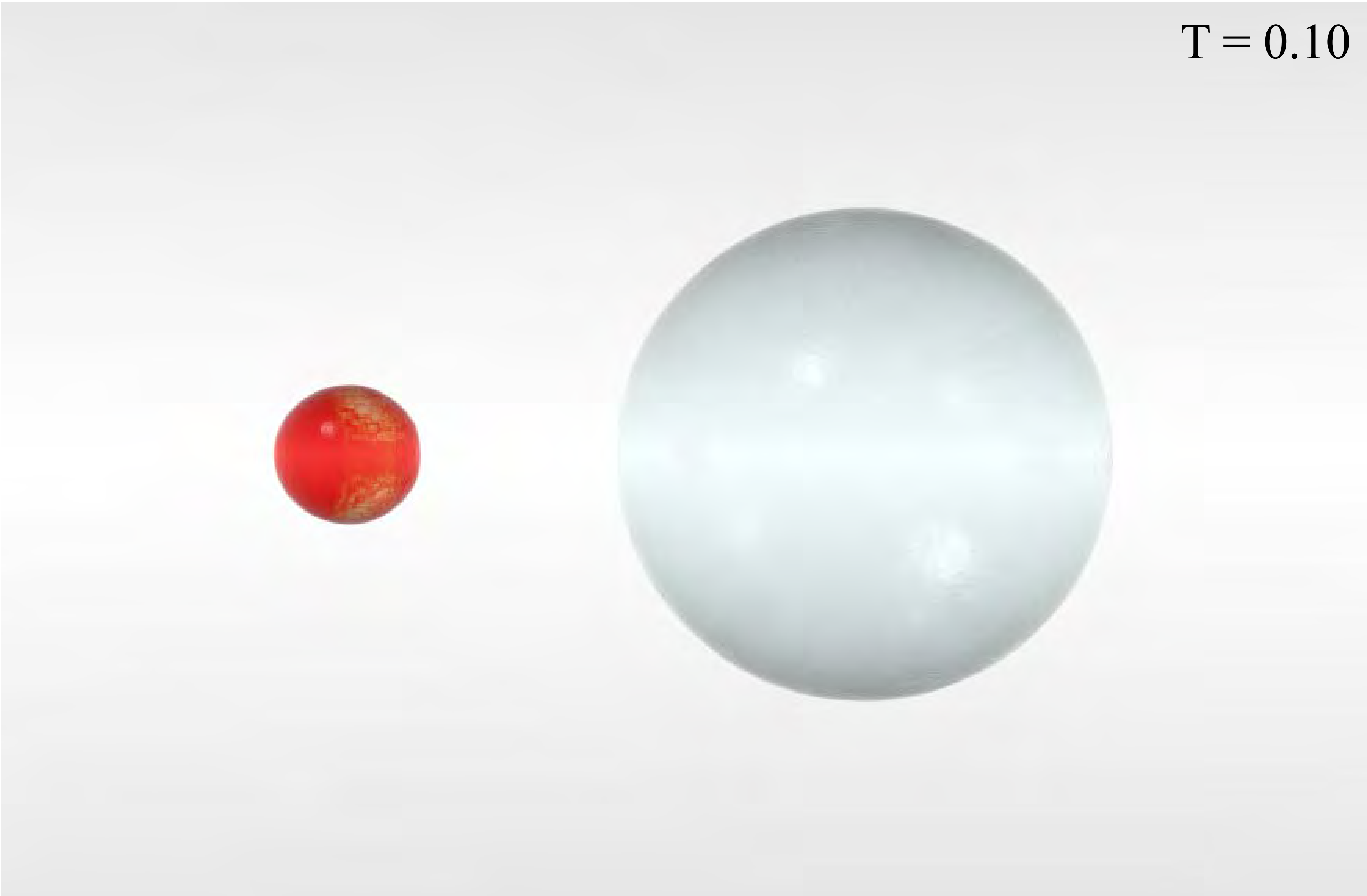
School of Aerospace Engineering



Unequal Coalescence Collision

Movie

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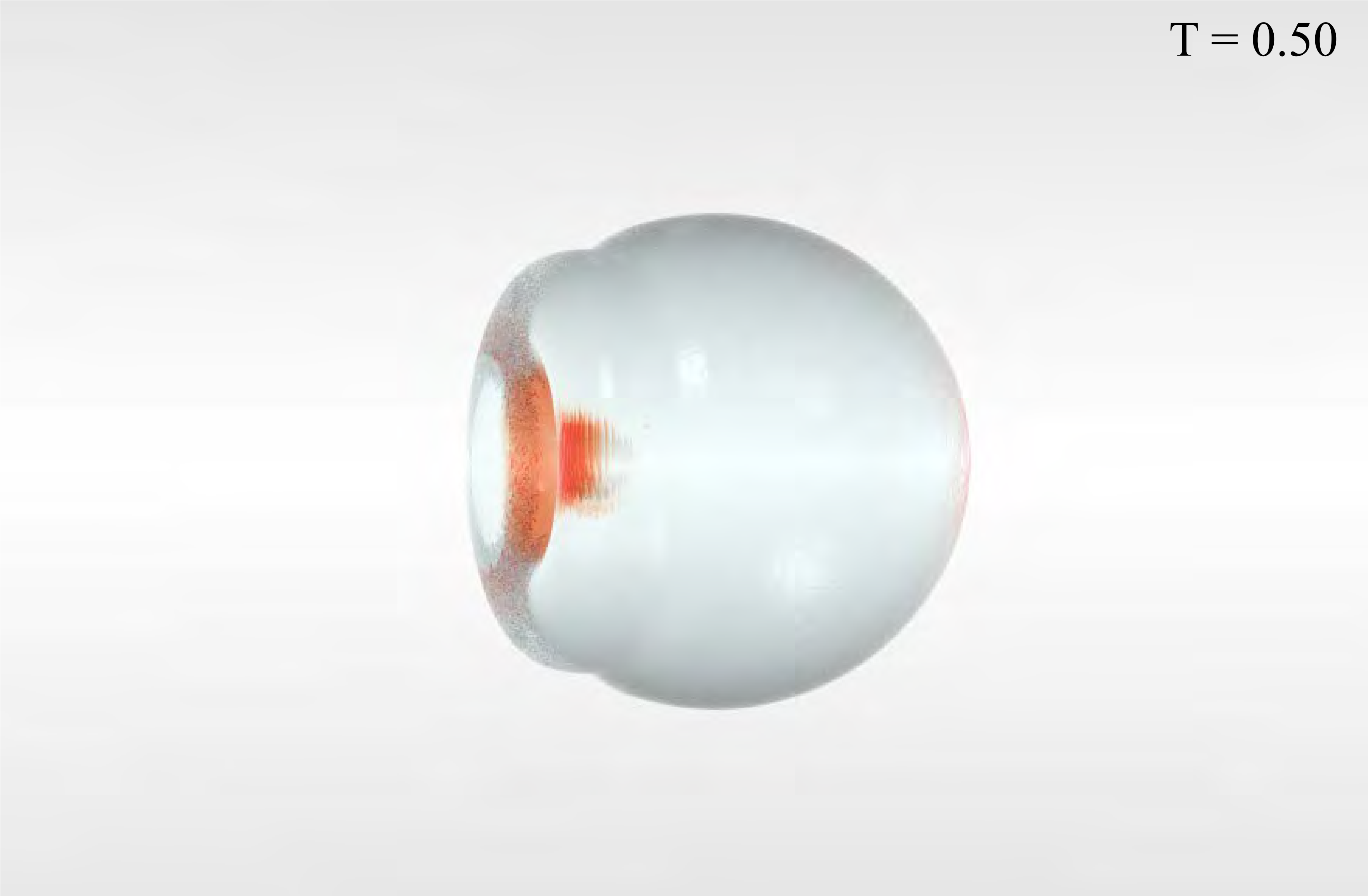
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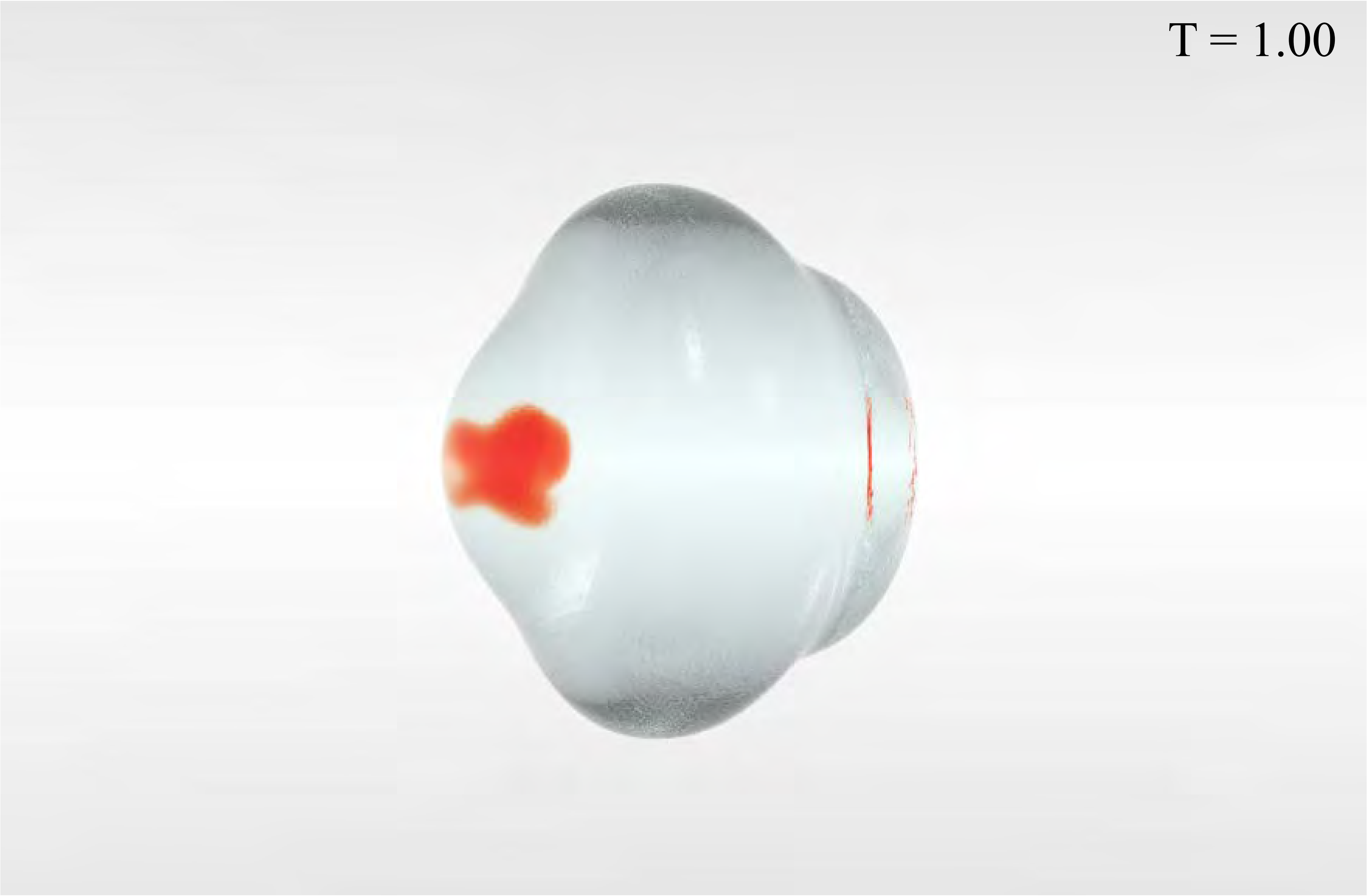
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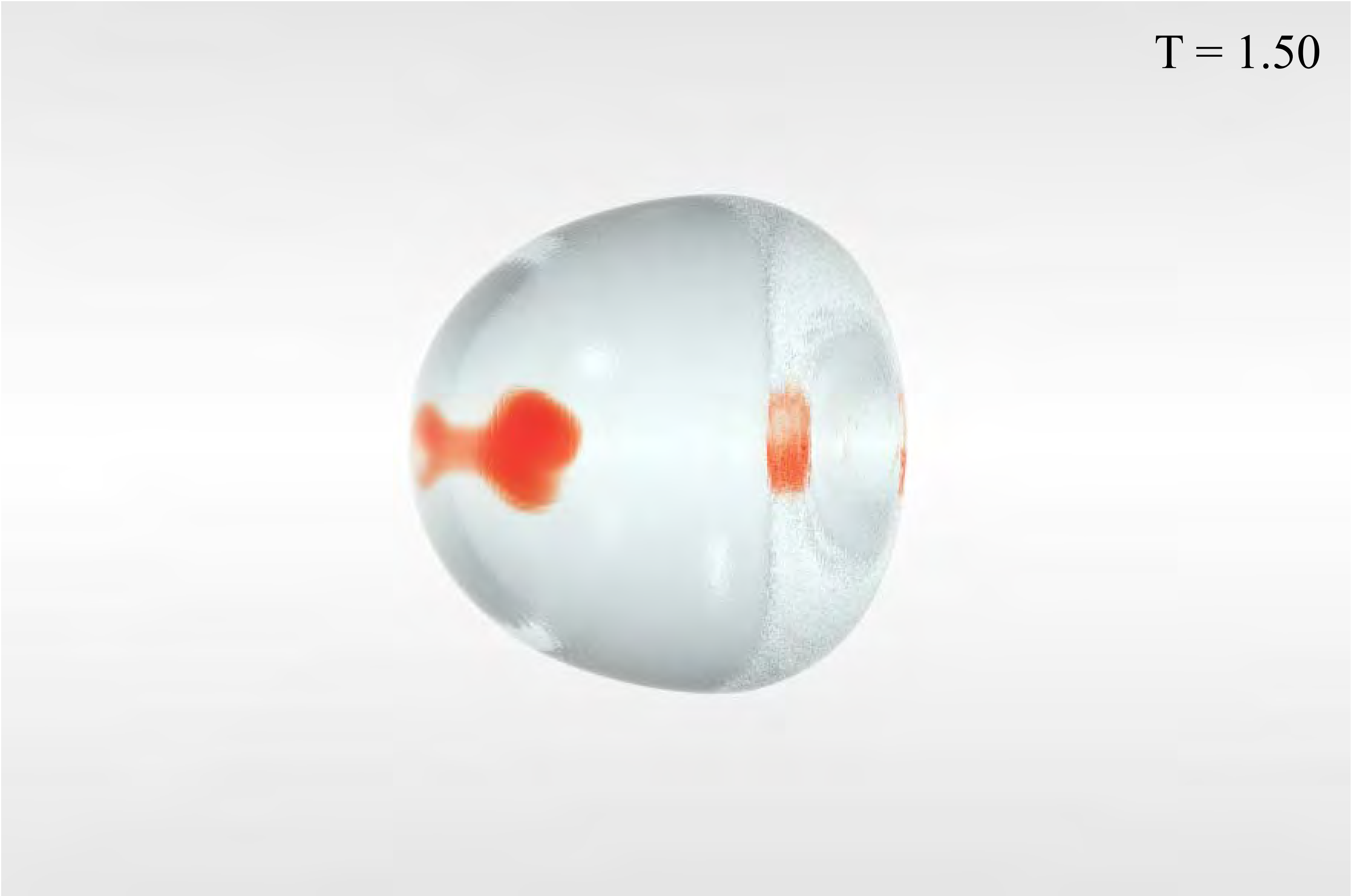
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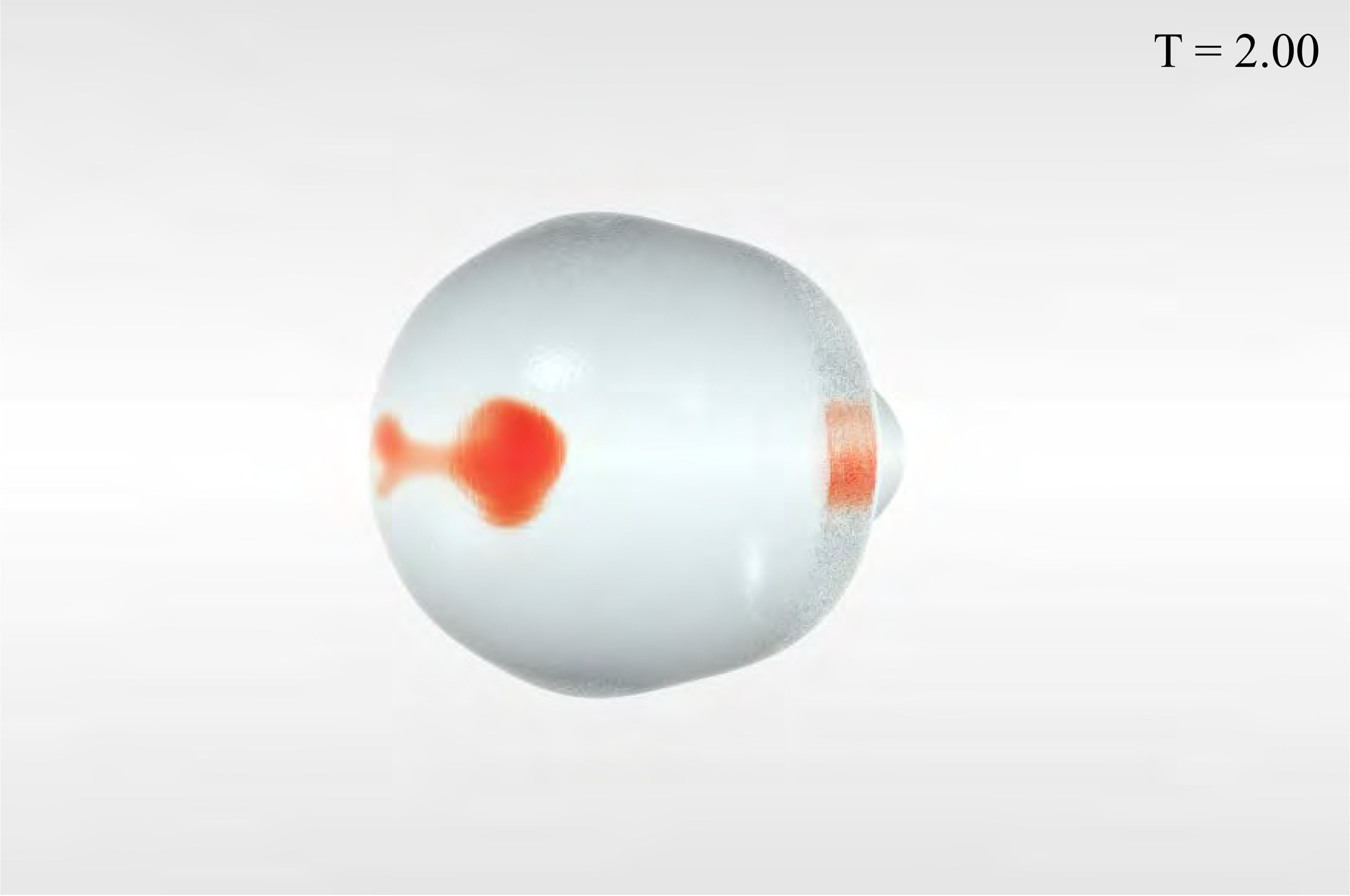
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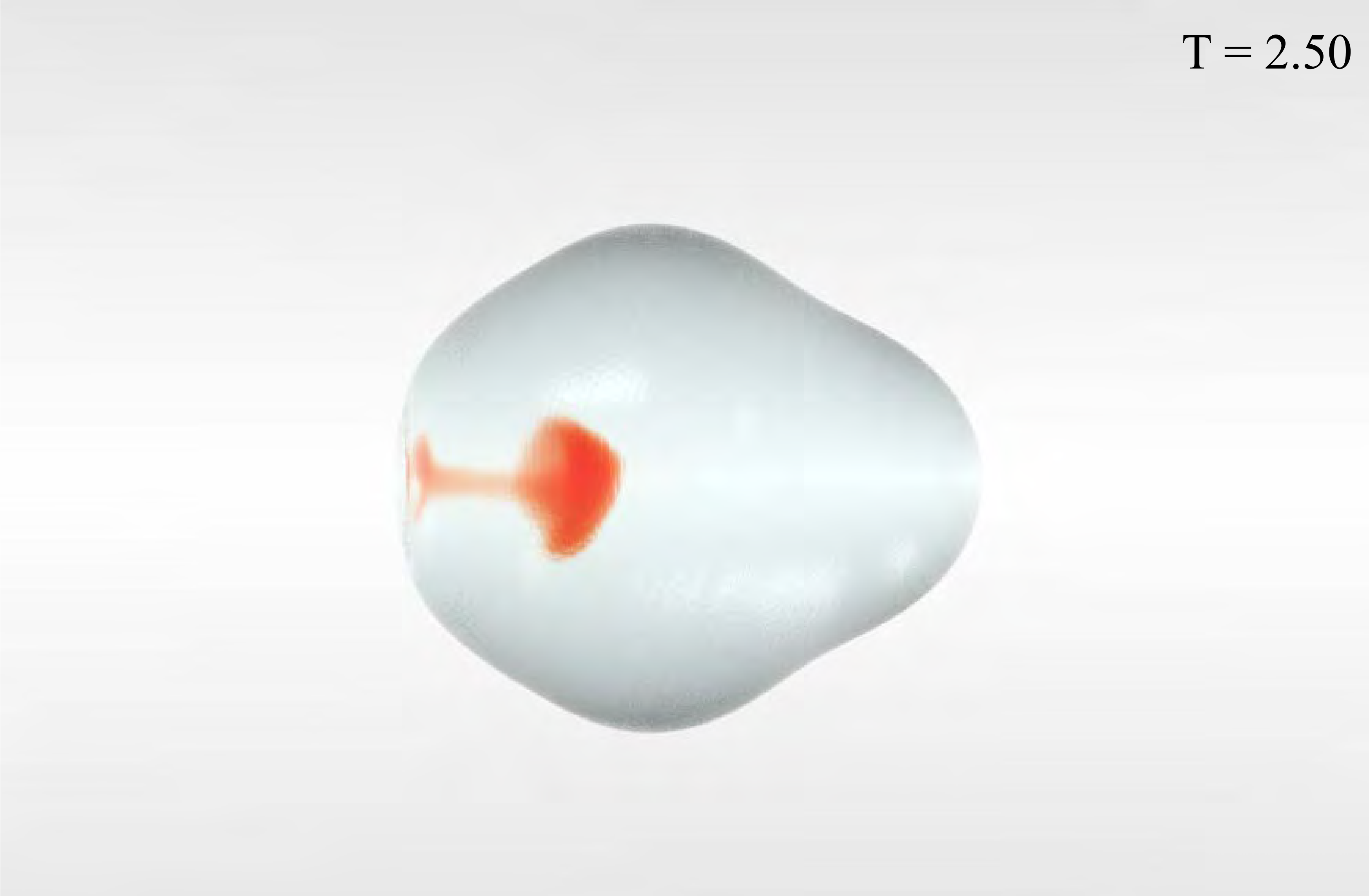
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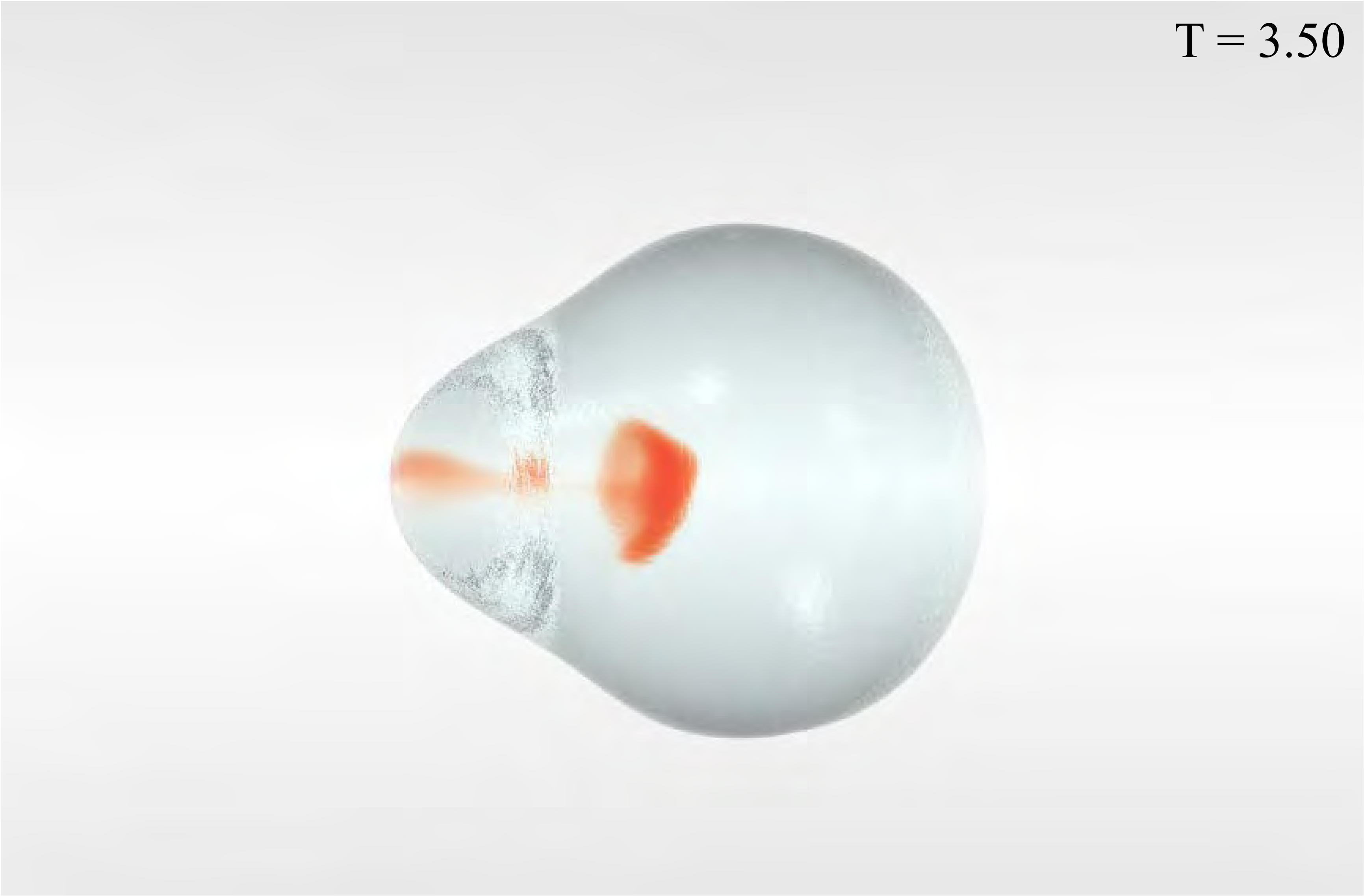
T = 3.00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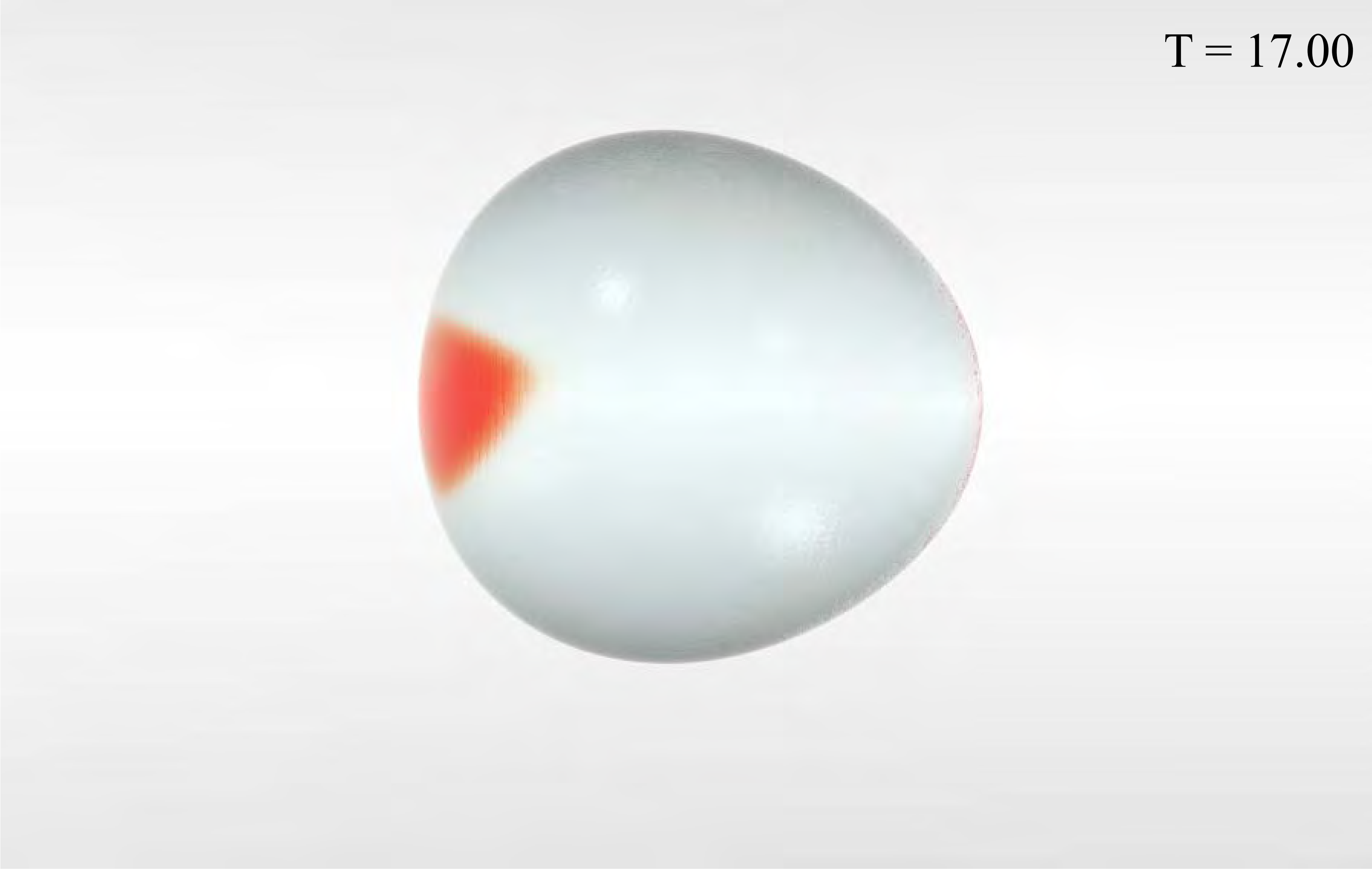
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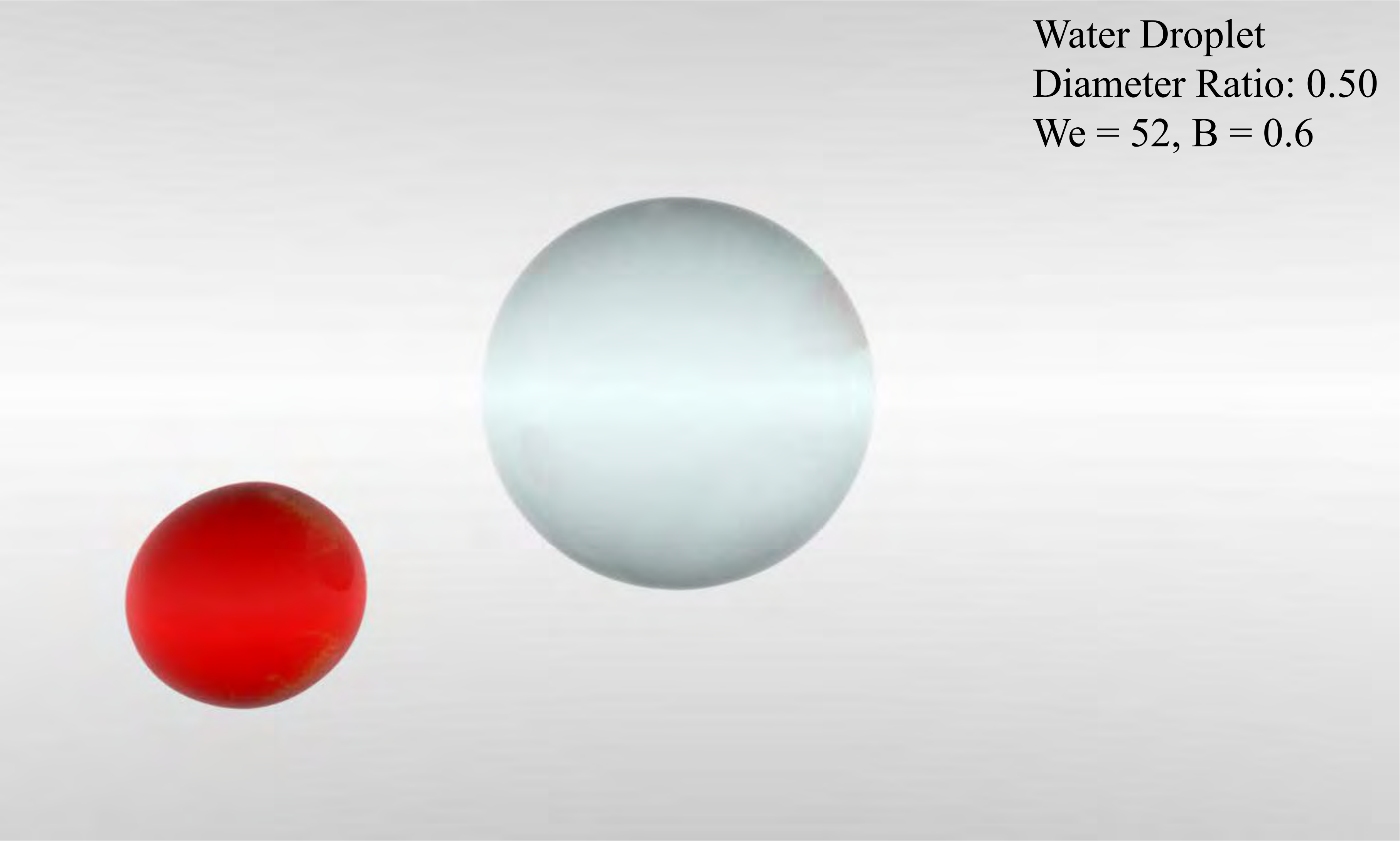
Unequal Stretching Separation



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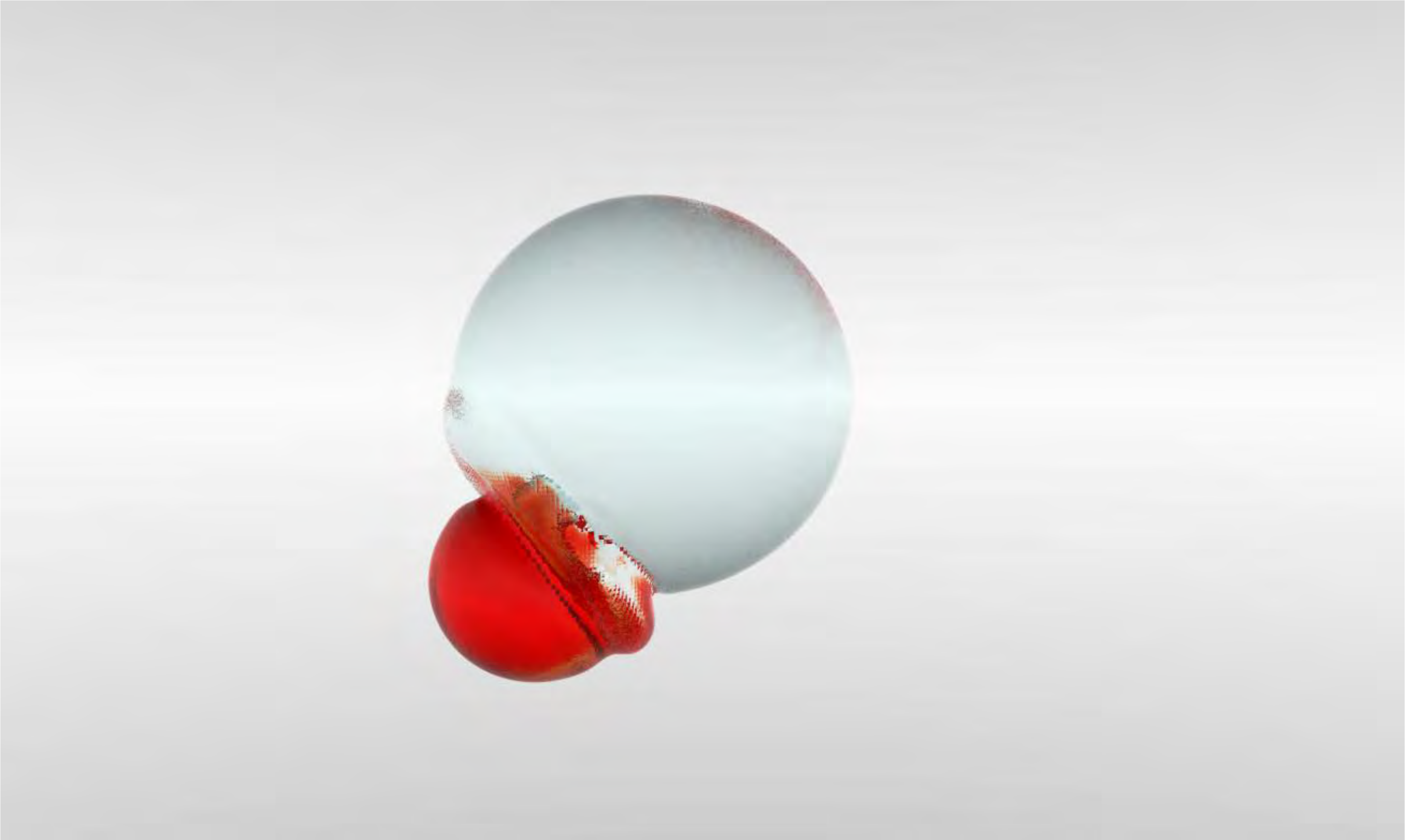

Unequal Stretching Separation

Unequal Stretching Separation

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Unequal Stretching Separation

Unequal Stretching Separation

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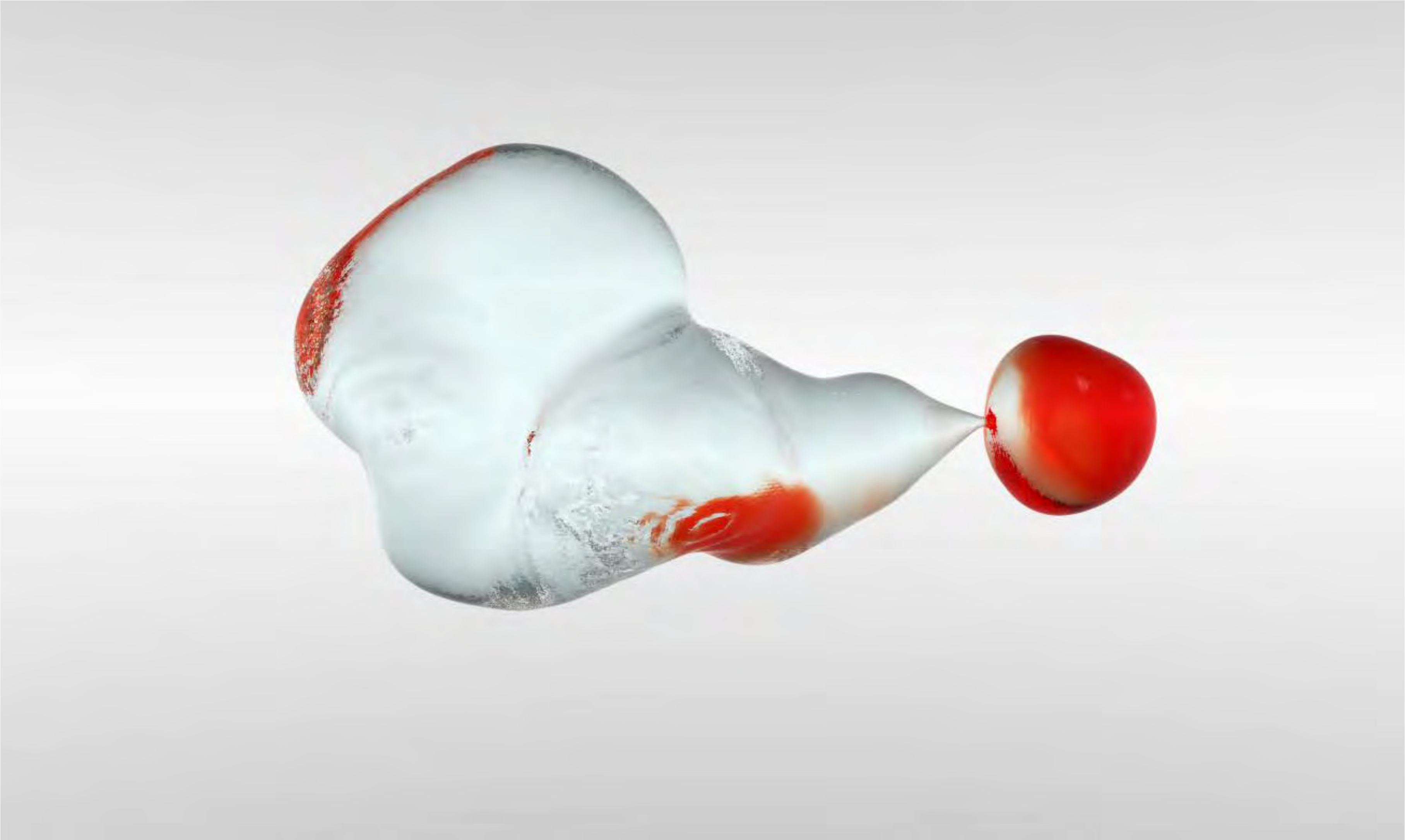
Unequal Stretching Separation



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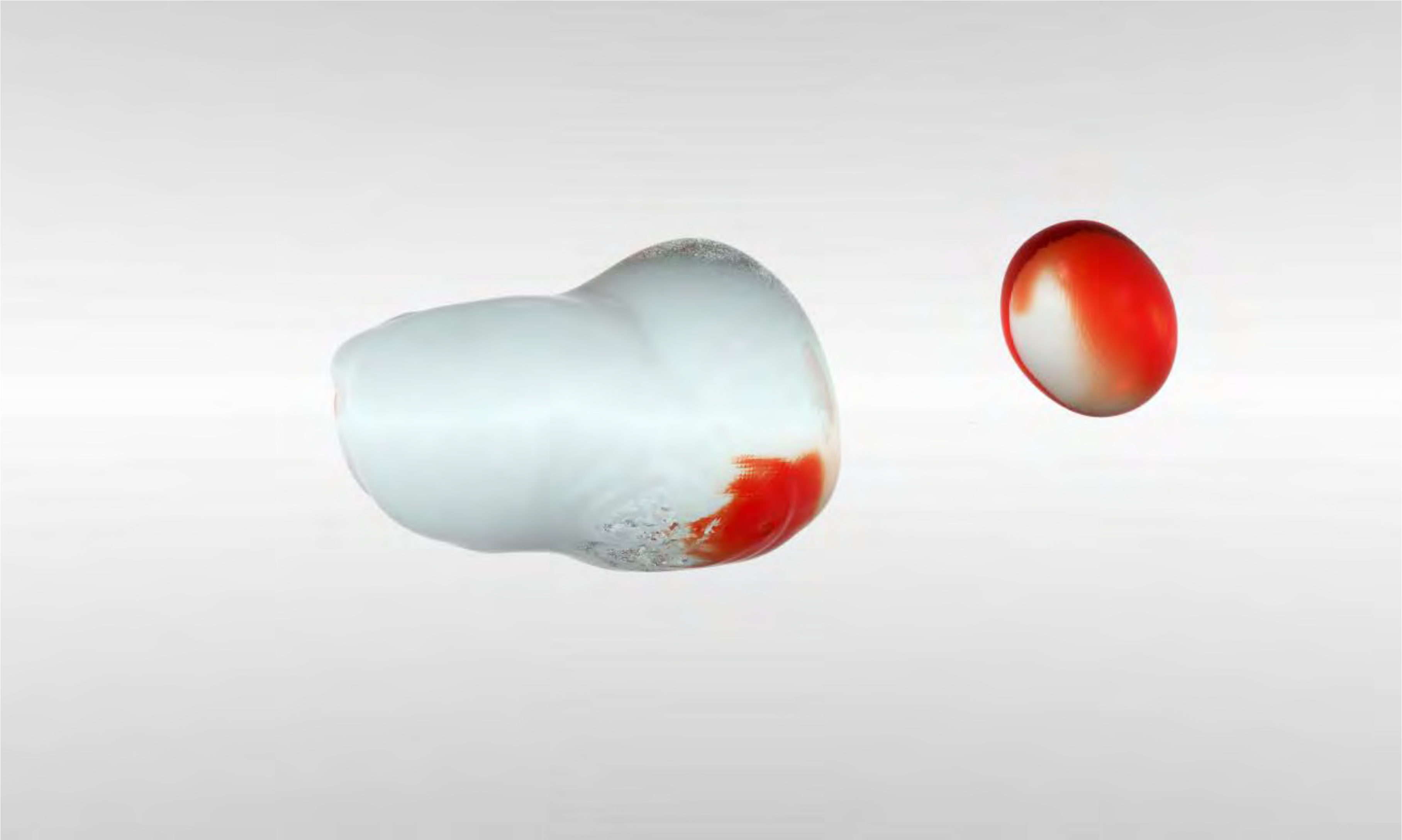


Two-Stage Interfacial Reactions

Stage One:

Transform liquid phase where two droplets are in contact into gas phase

Stage Two:

Impose volume source at the interface

Since new volume is generated by chemical reaactions, volume sources or sinks should be found at the interface. An obvious approach is

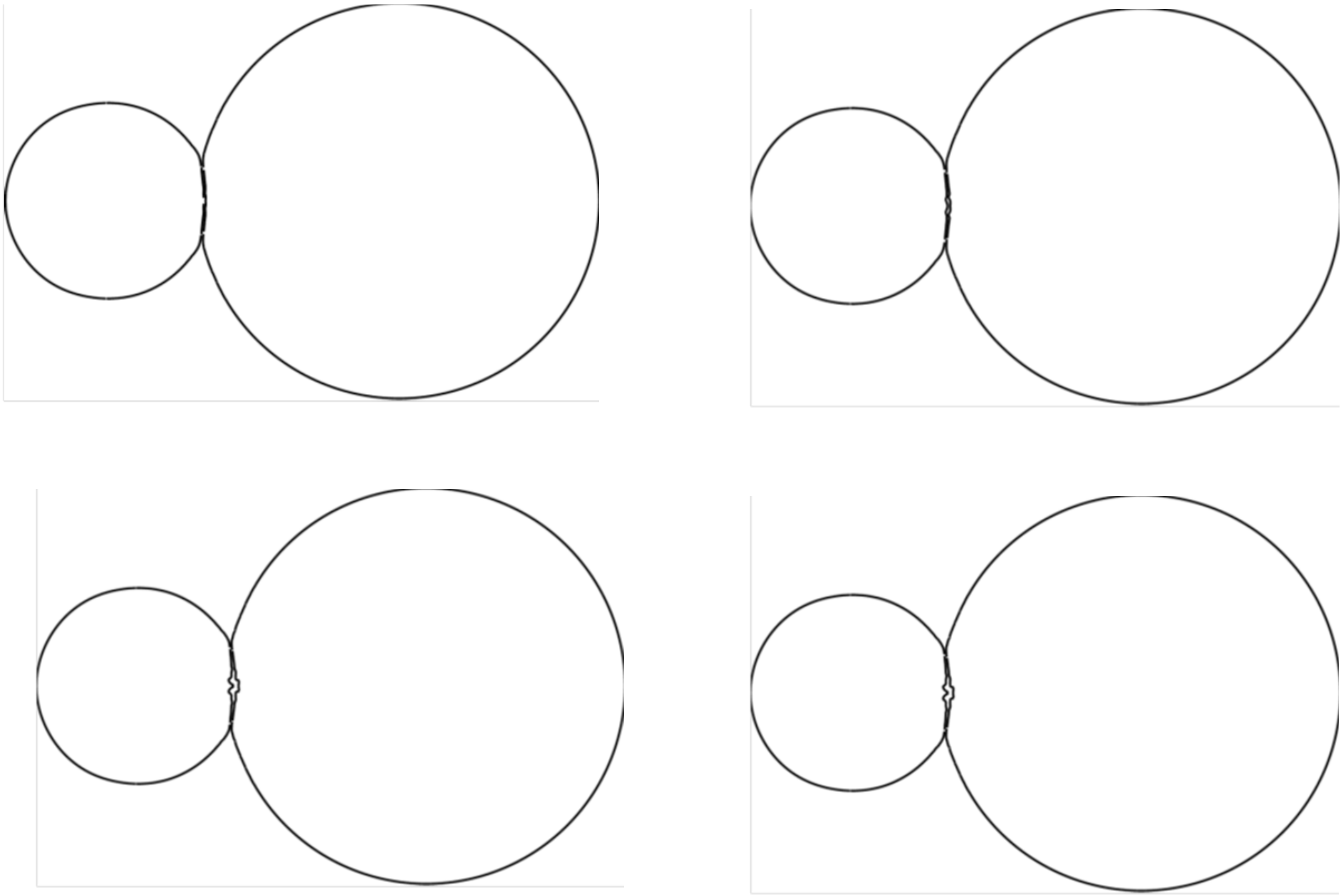
$$\nabla \cdot \mathbf{u} = \dot{m}\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right)$$

where $\dot{m}$ is the volumetric mass source of gas. A volume balance is given on the right hand side.

Ref: Direct numerical simulation of evaporating droplets, JCP 2008

Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation



Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation

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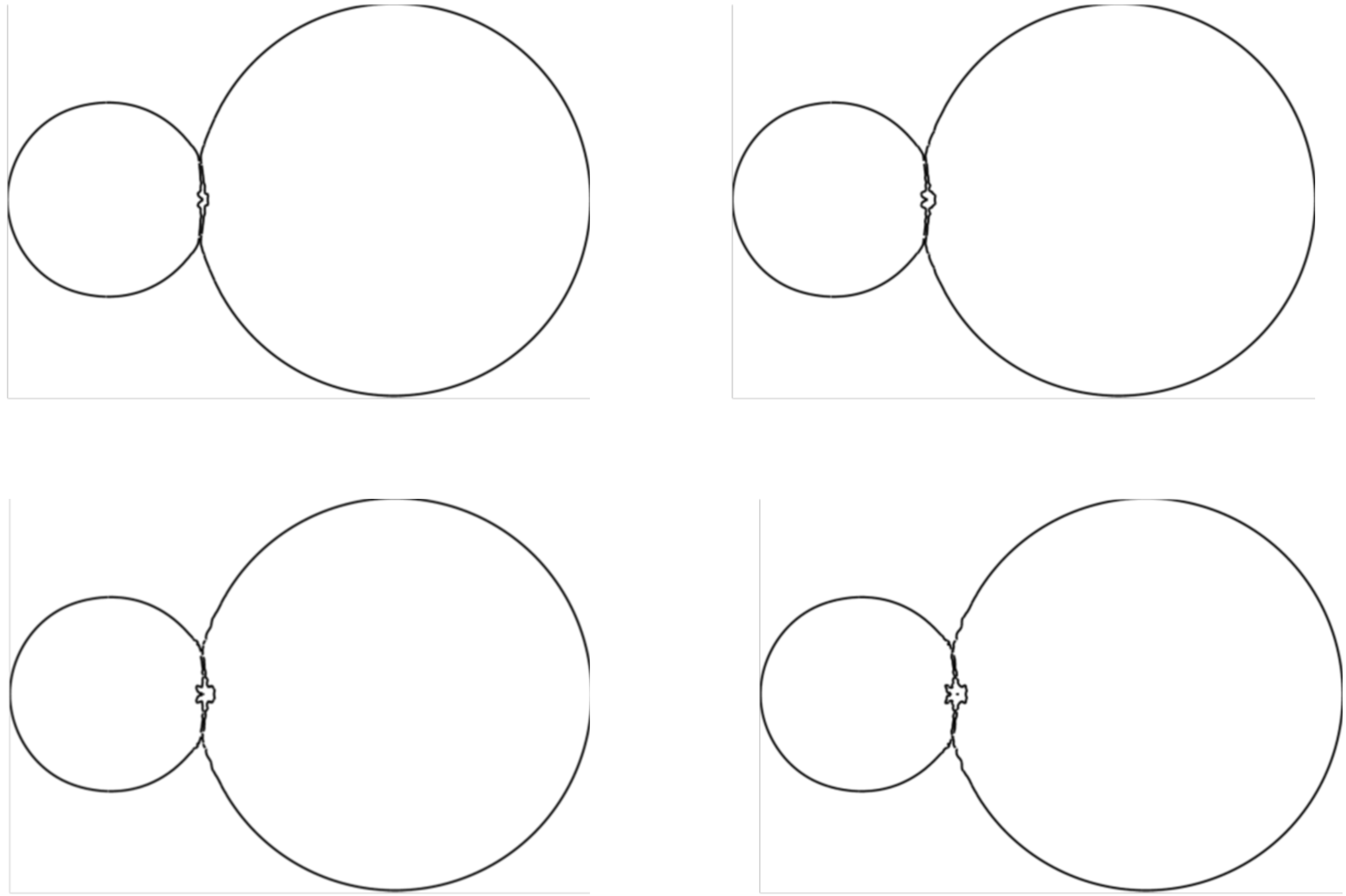
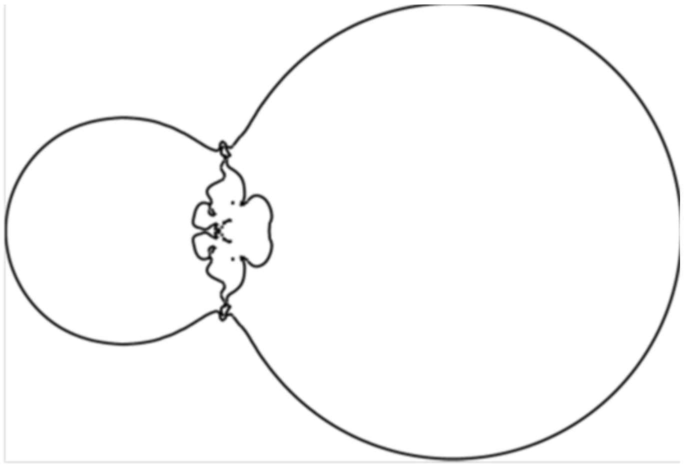
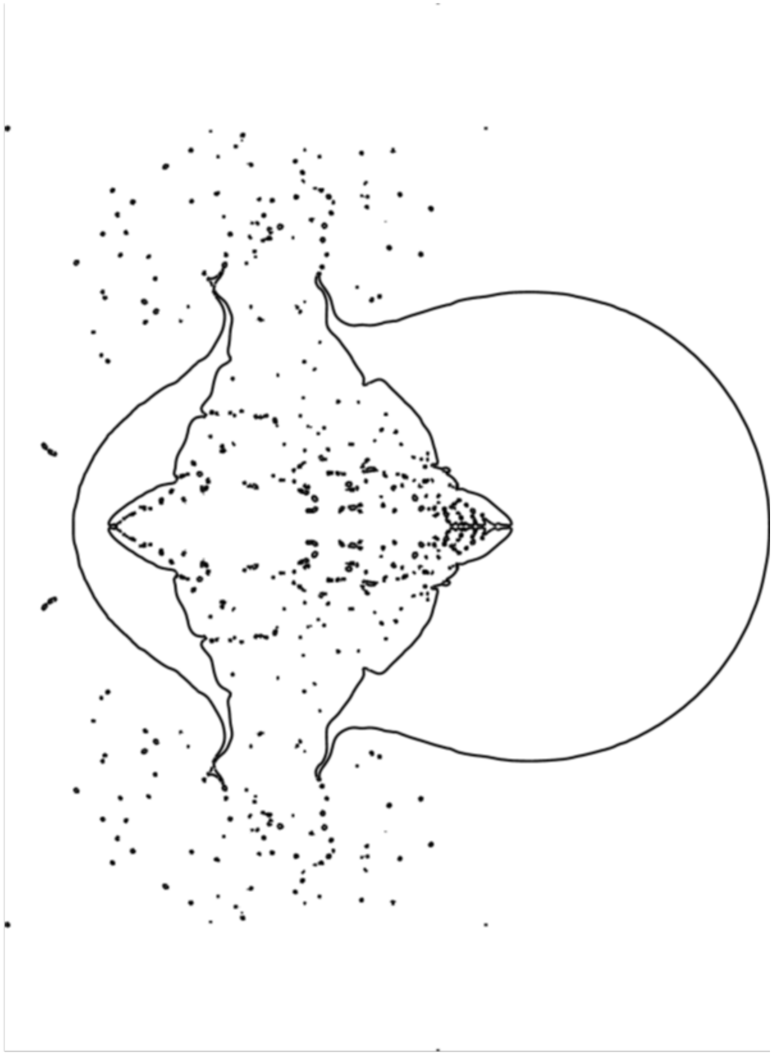


Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation





Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation

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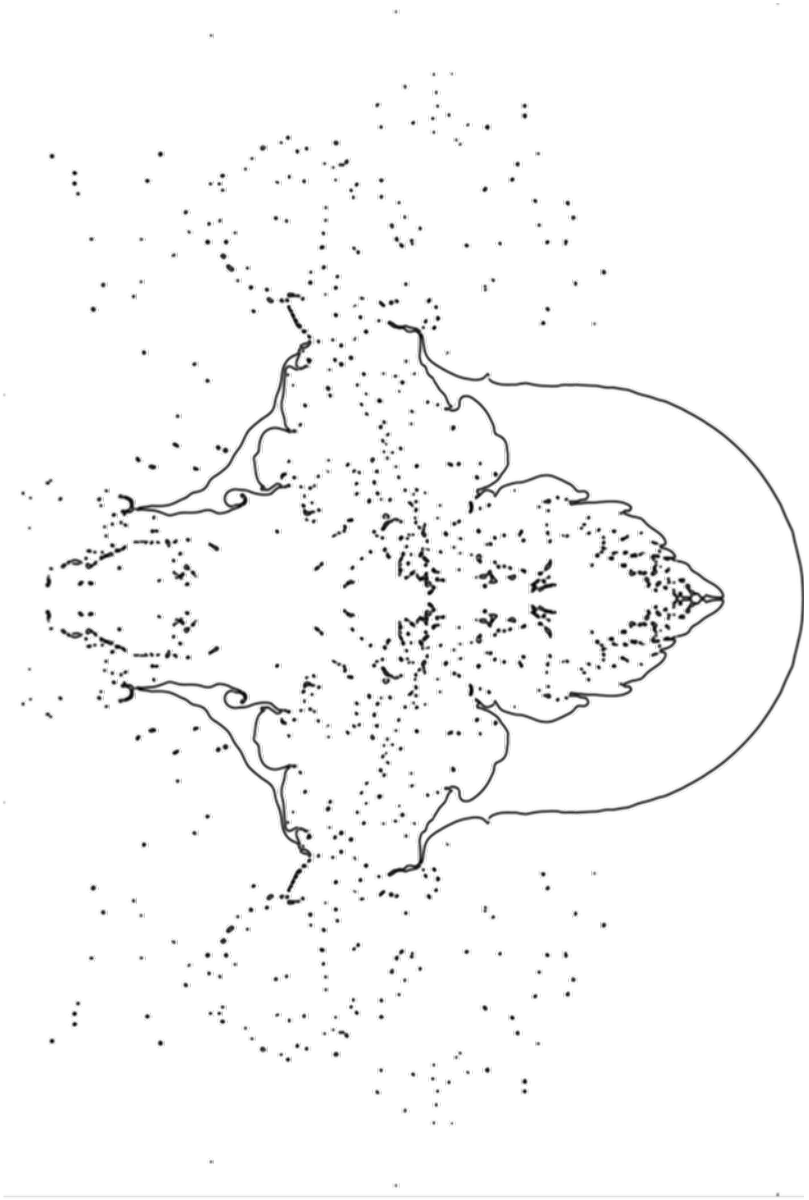
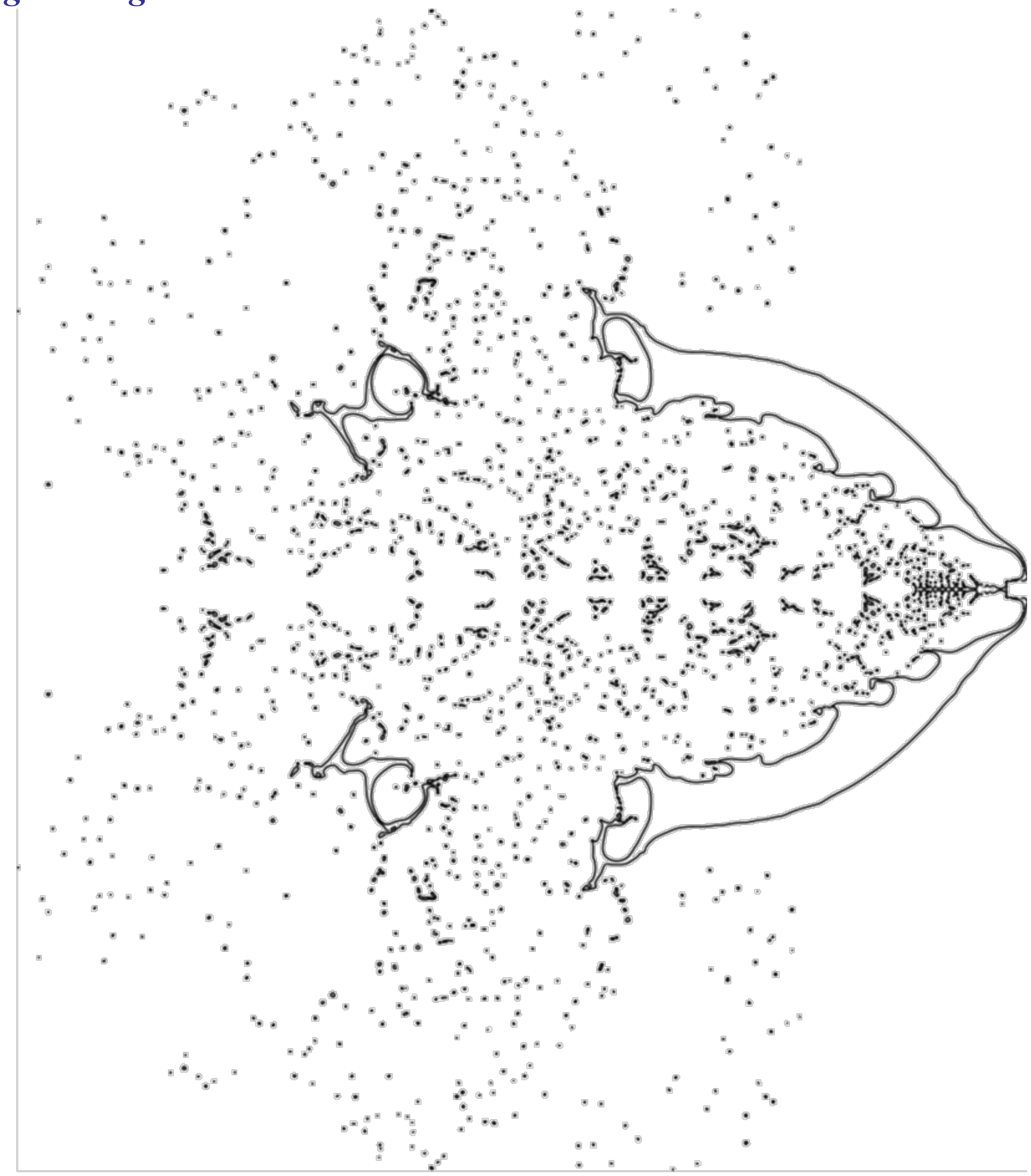


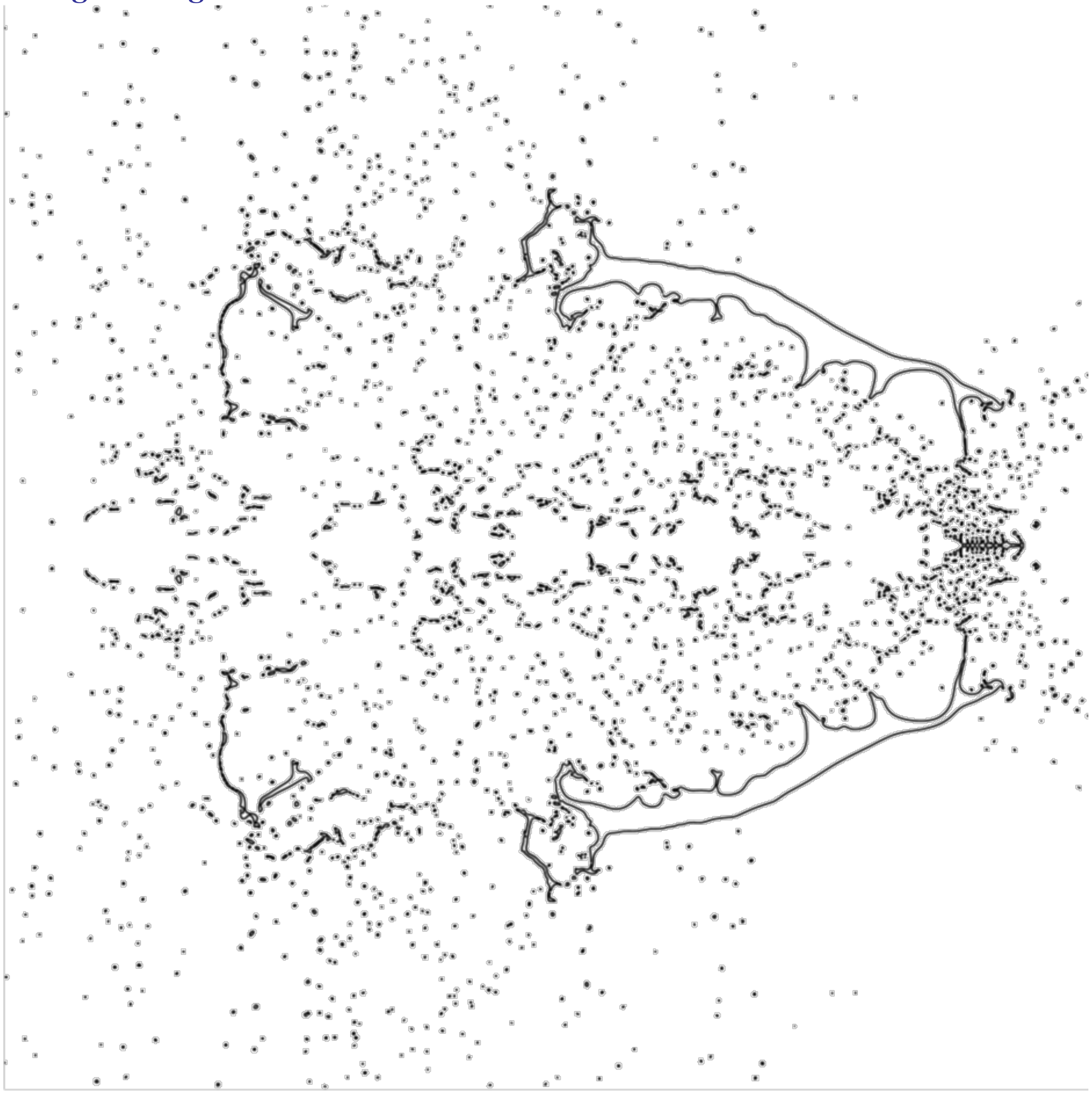
Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation



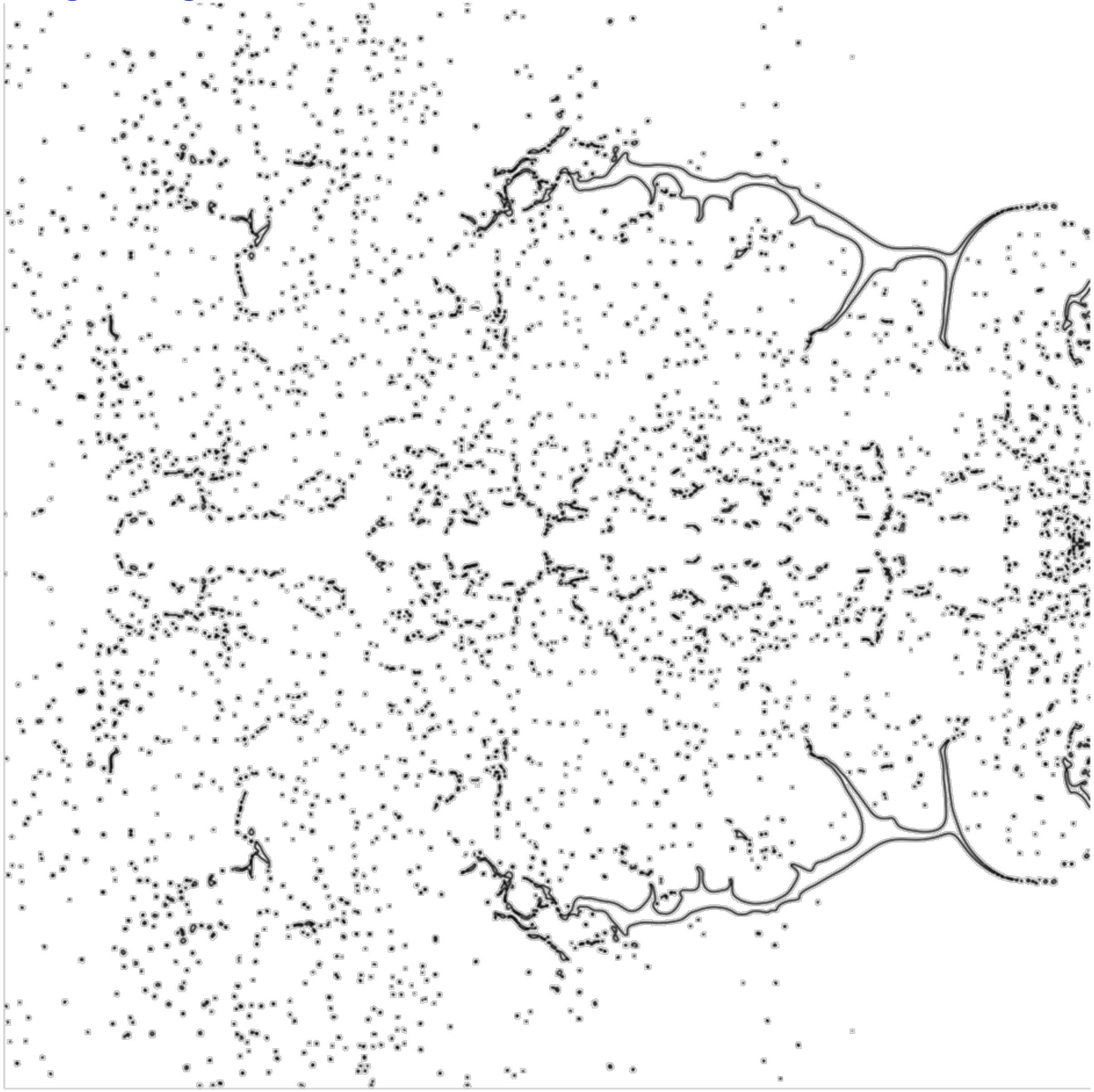
Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation



Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation



Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation

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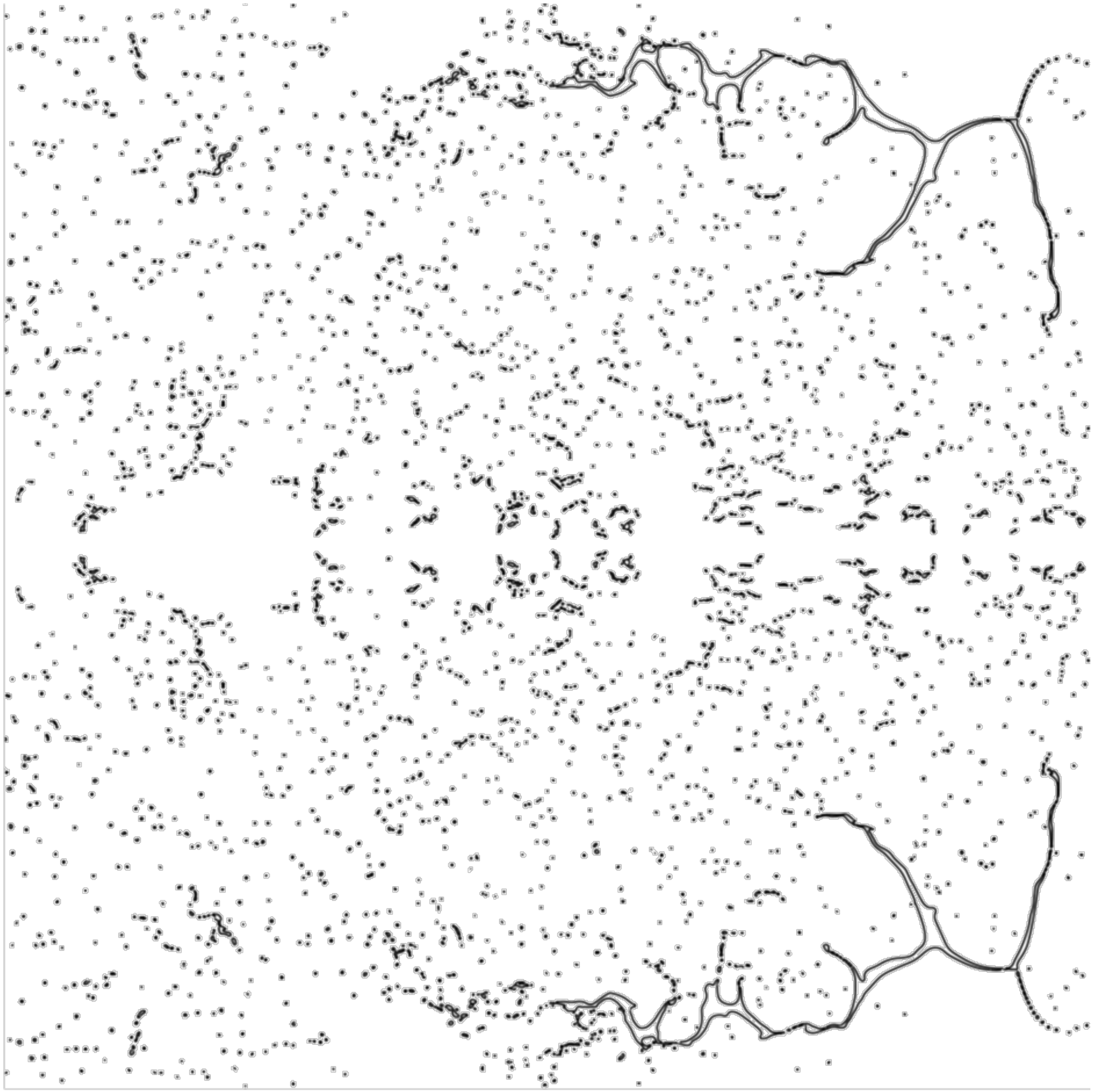
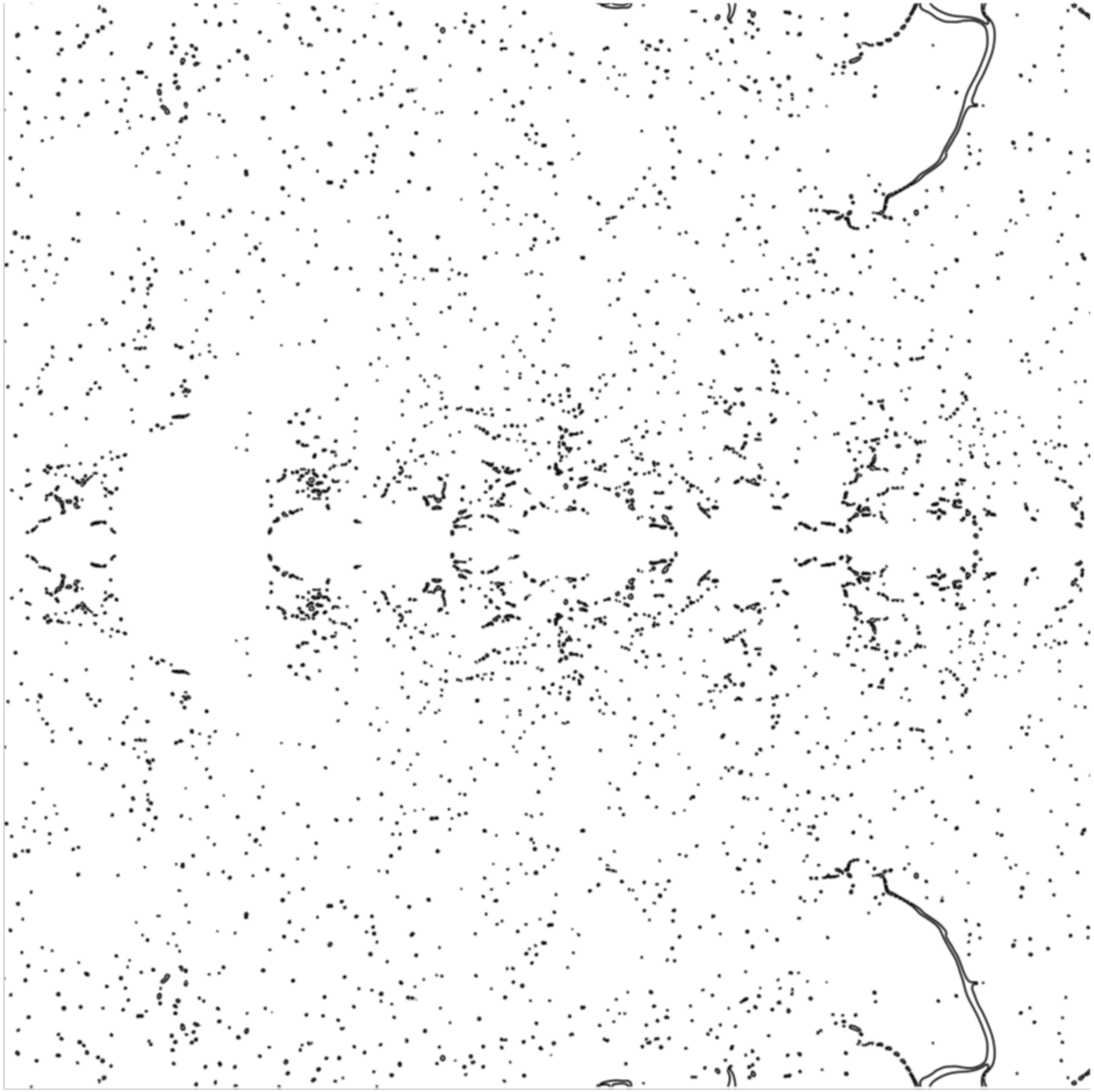


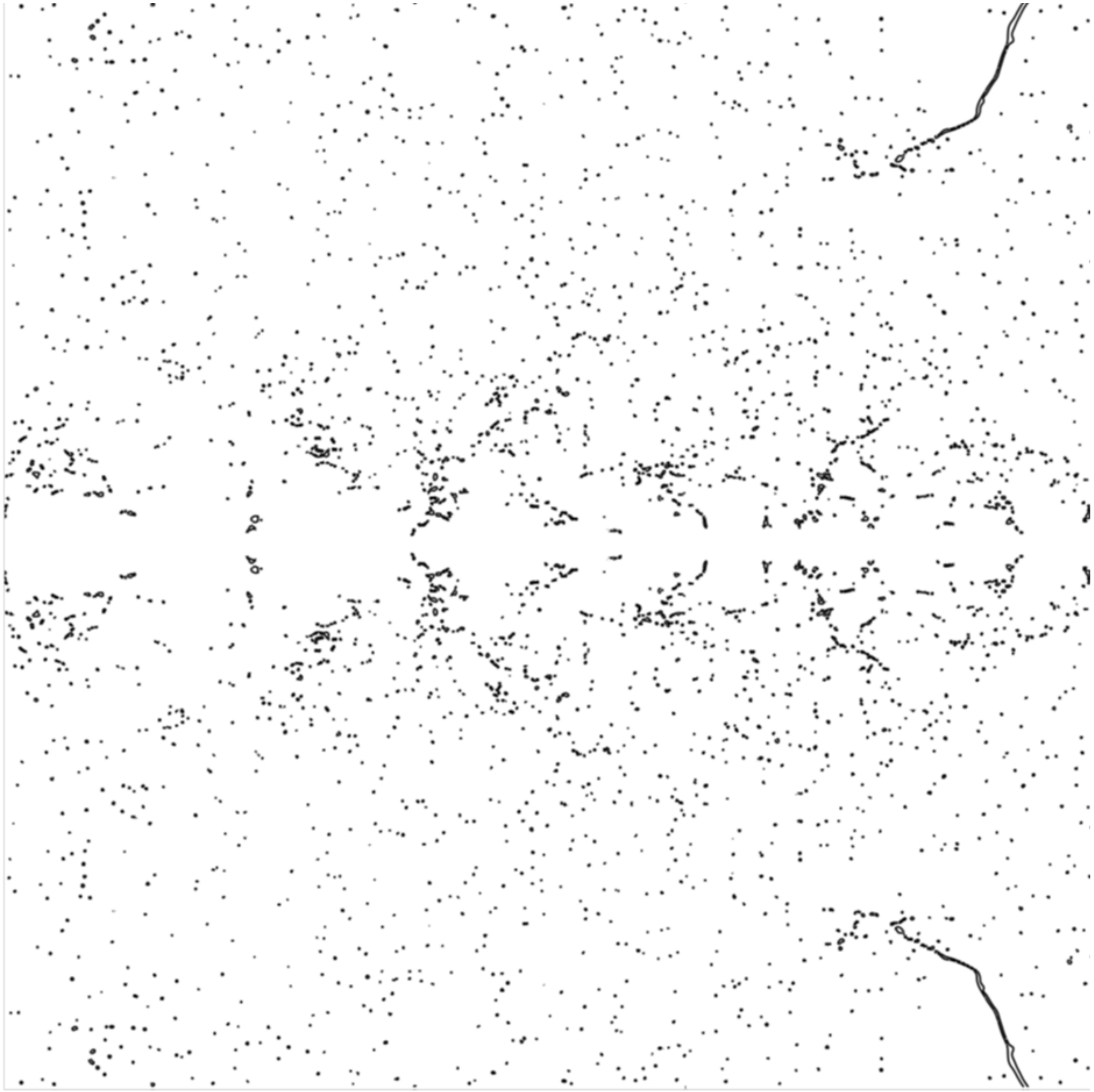
Droplet Collision with Interfacial Reaction

Axi-symmetric Simulation



Droplet Collision with Interfacial Reaction

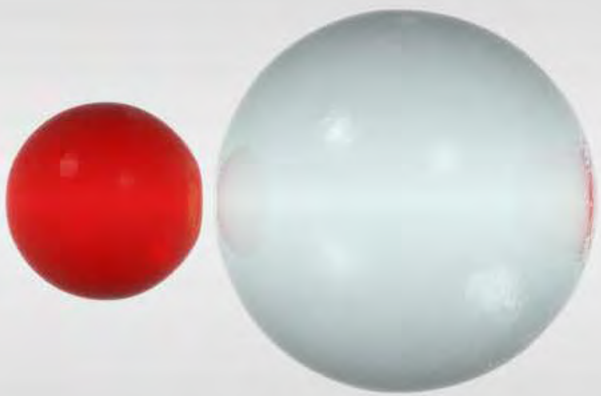
Axi-symmetric Simulation

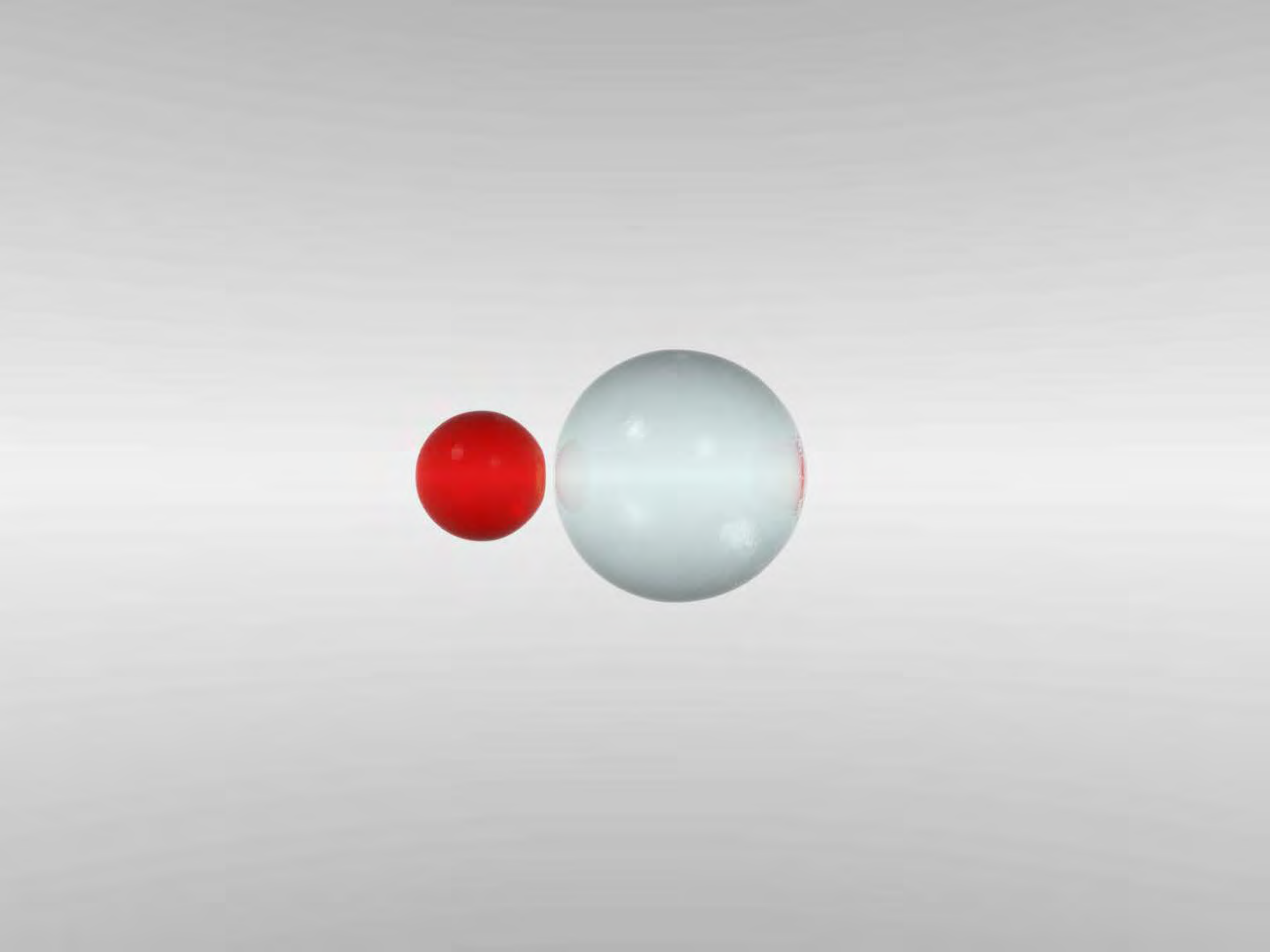


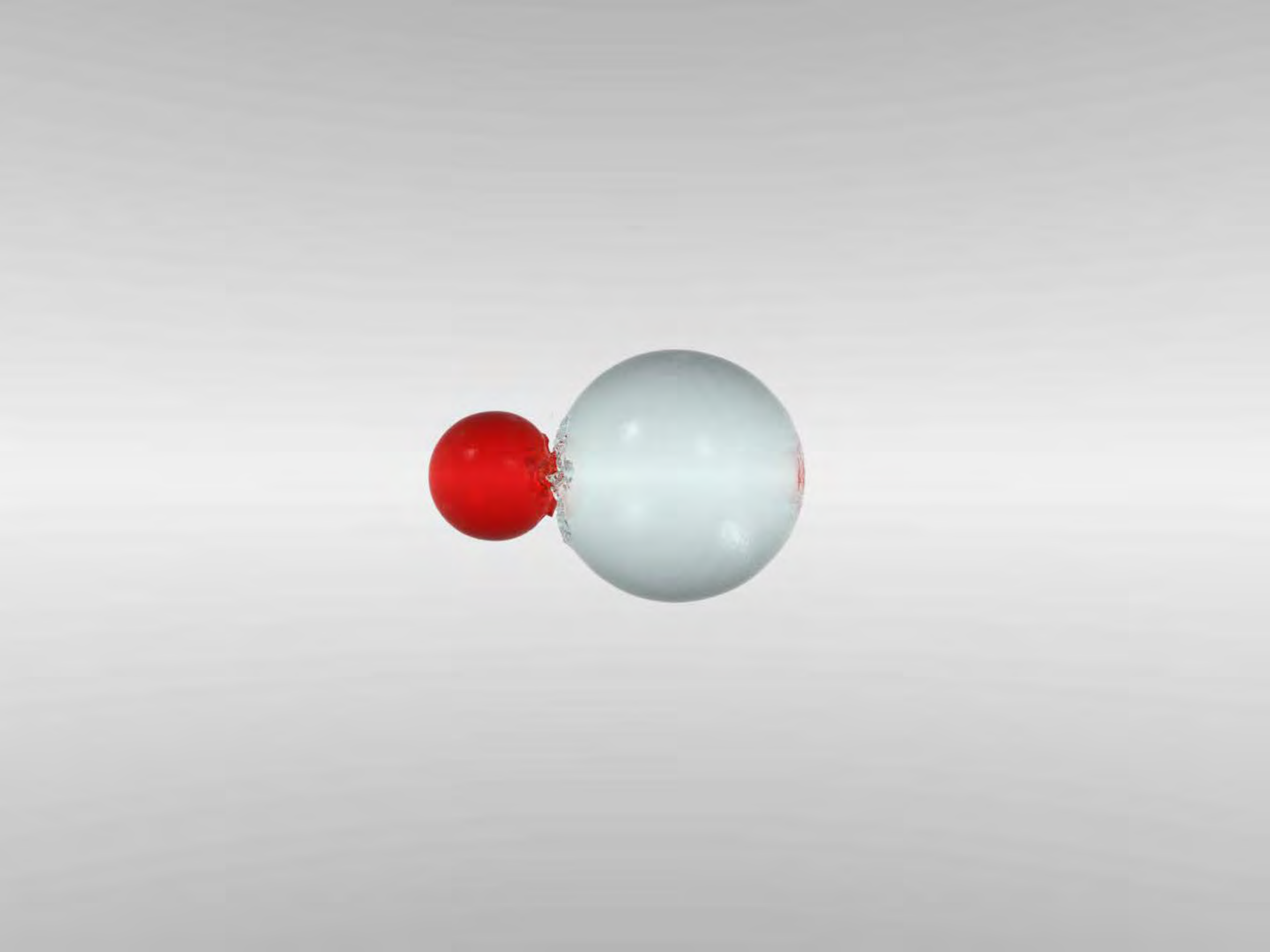
Droplet Collision with Interfacial Reaction

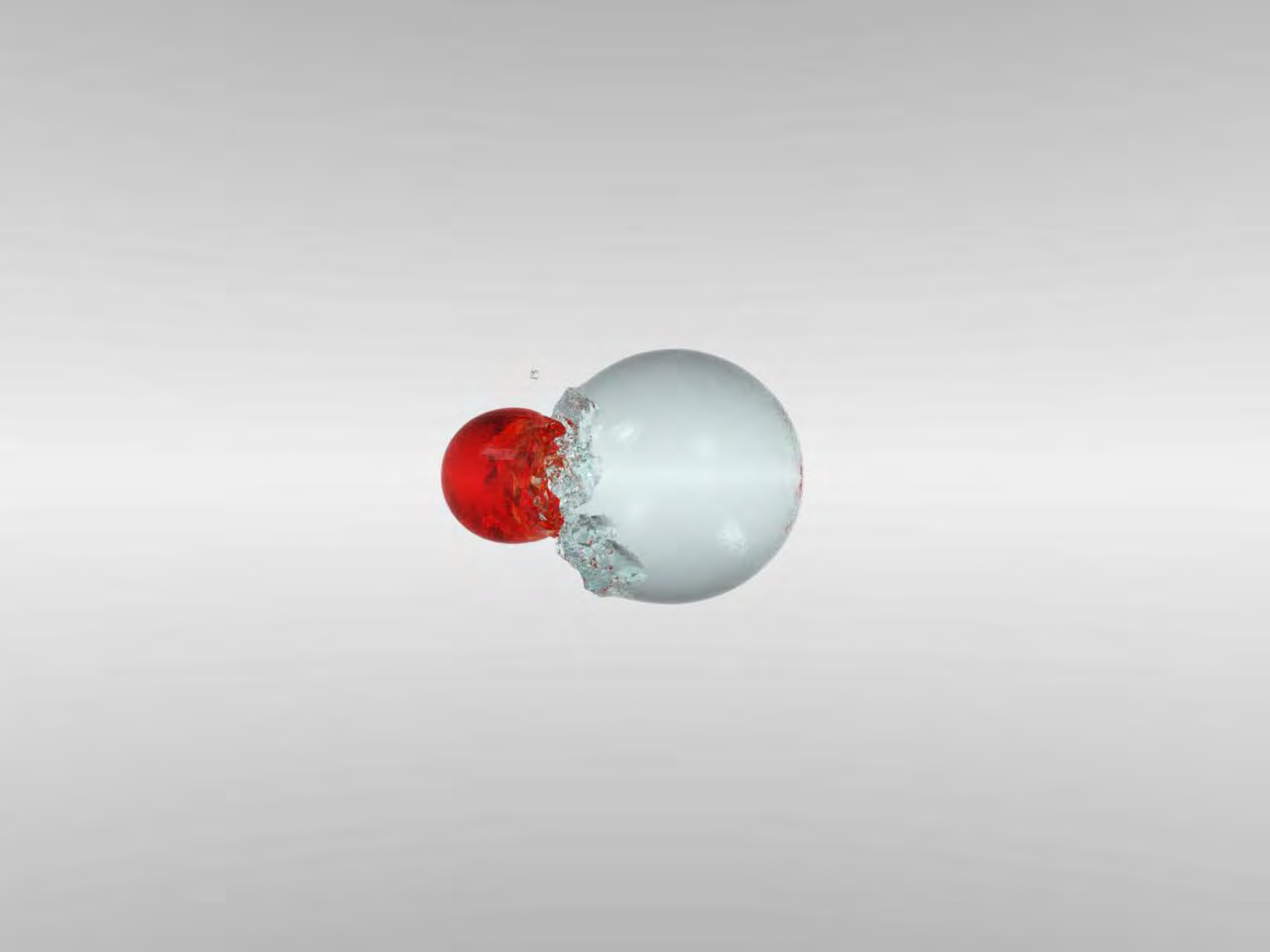
3-D simulation

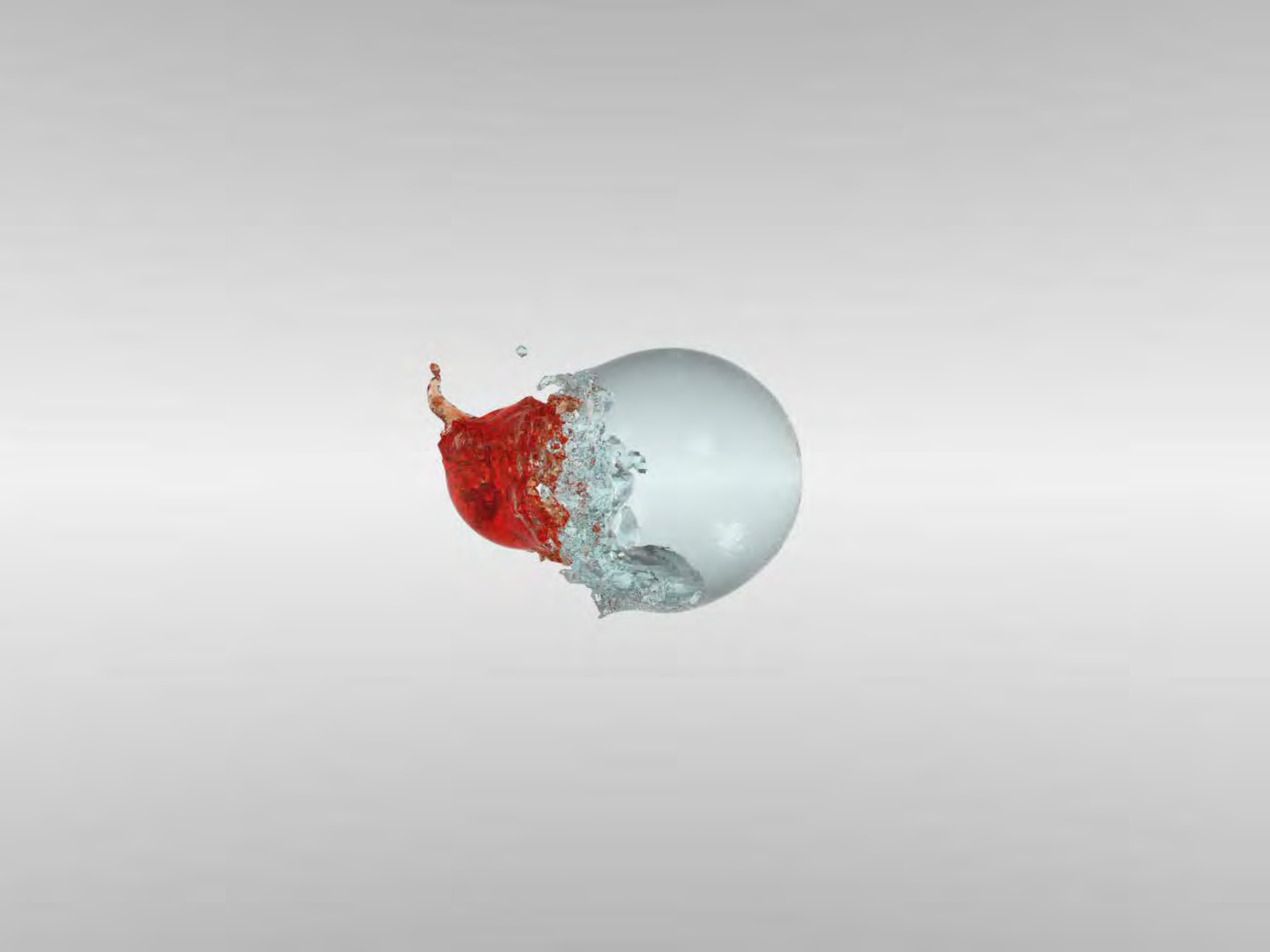
Movie

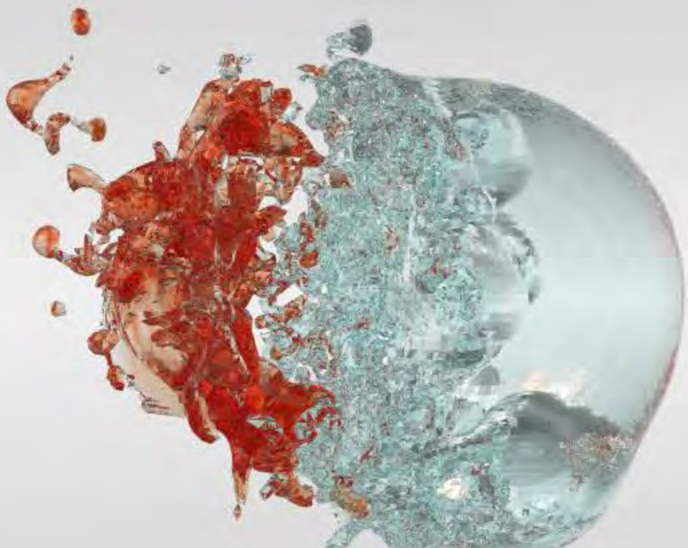


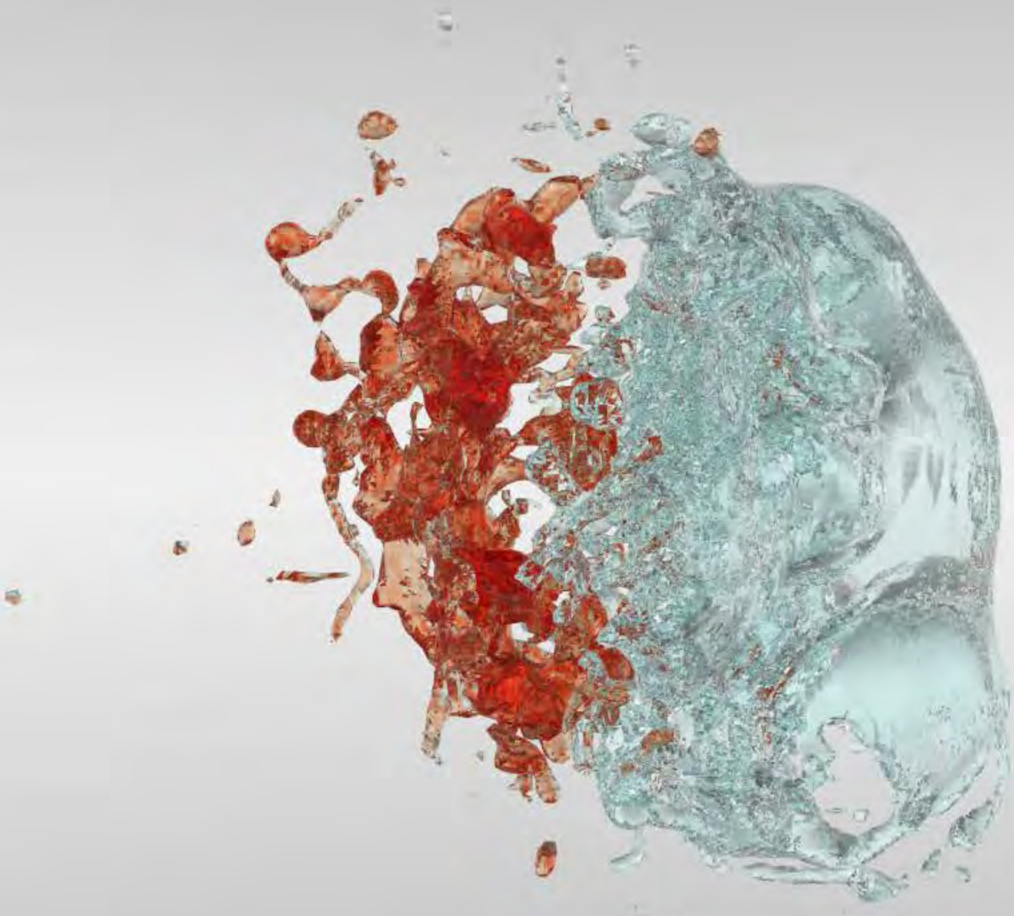


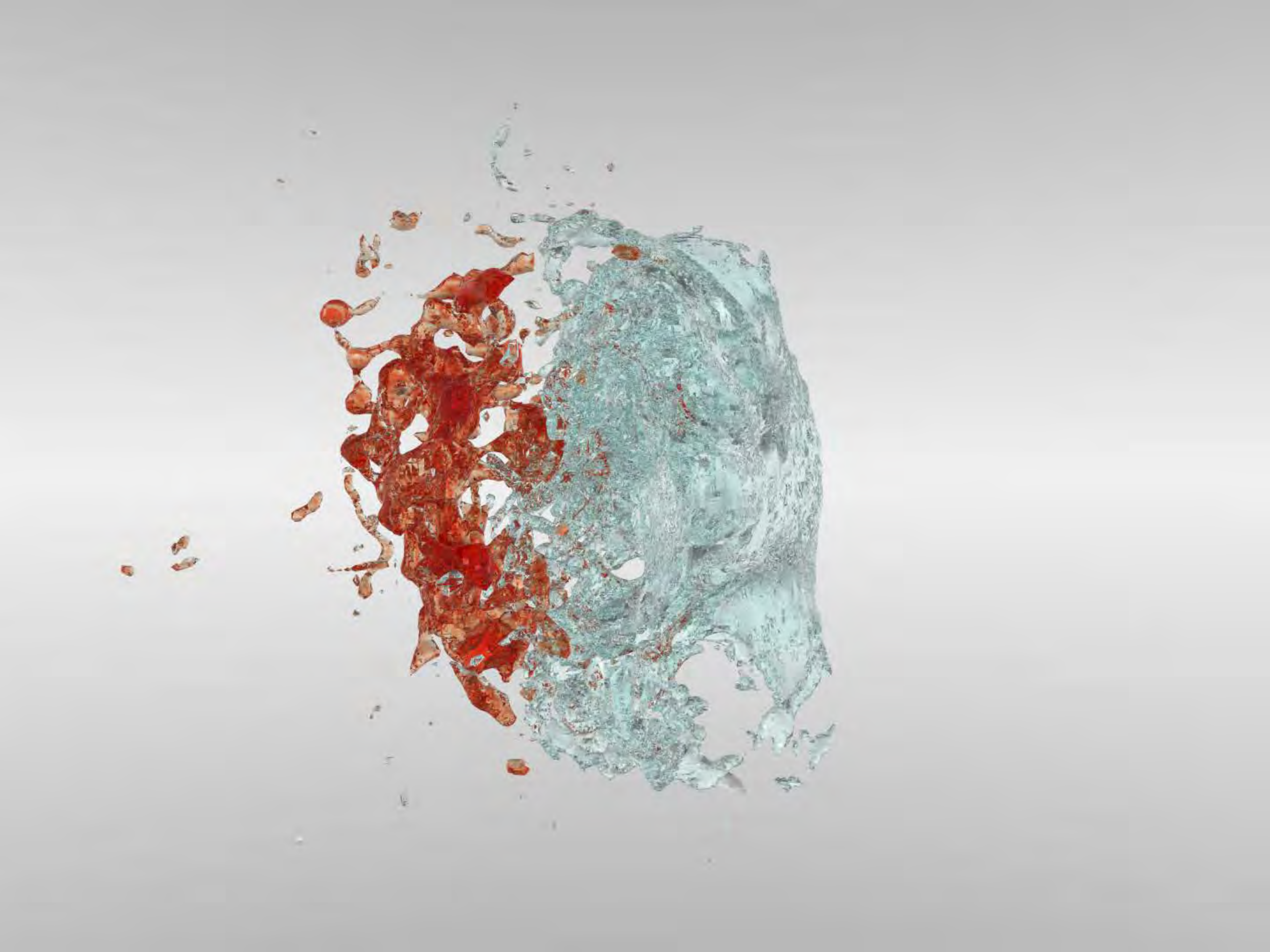


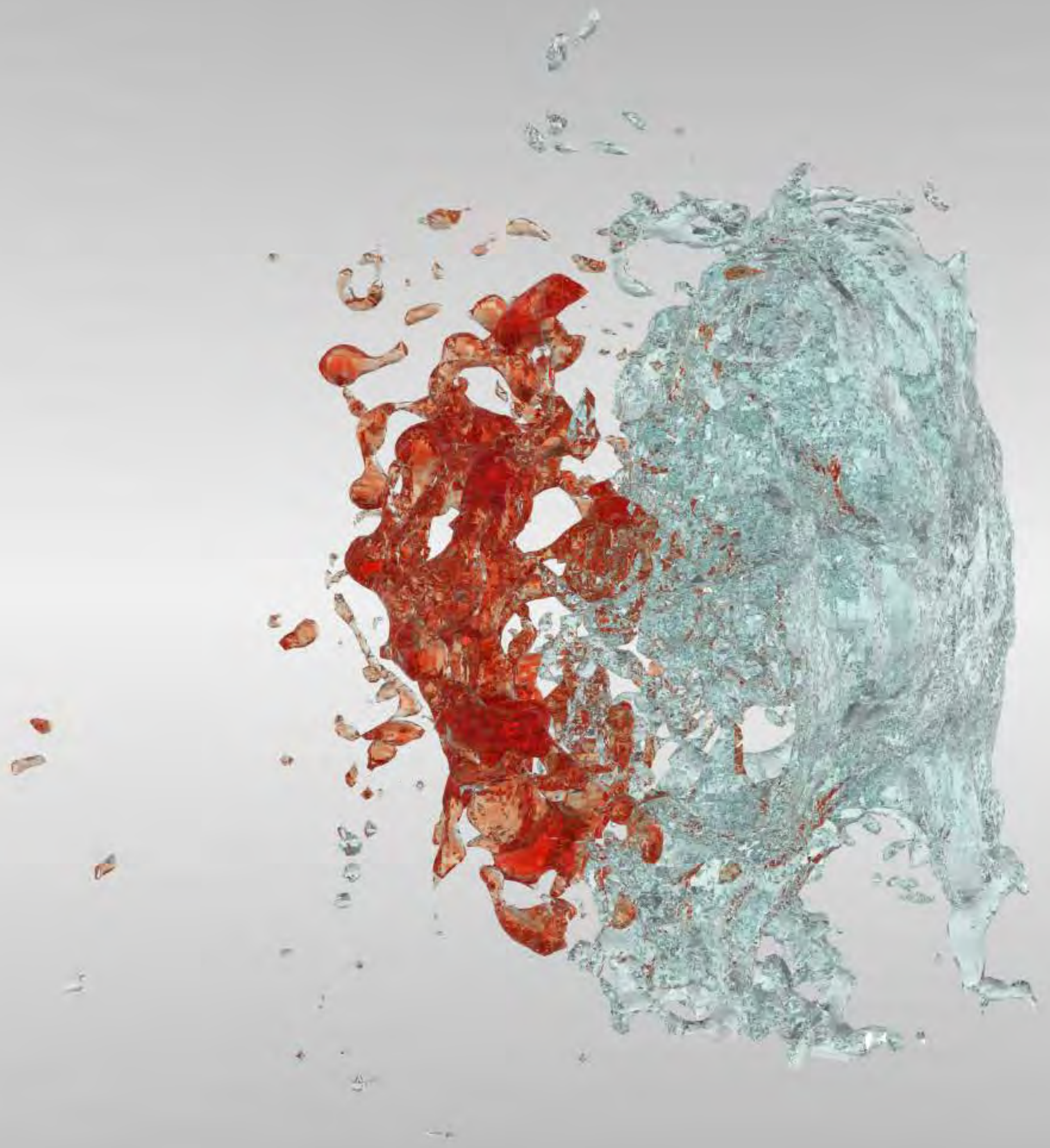


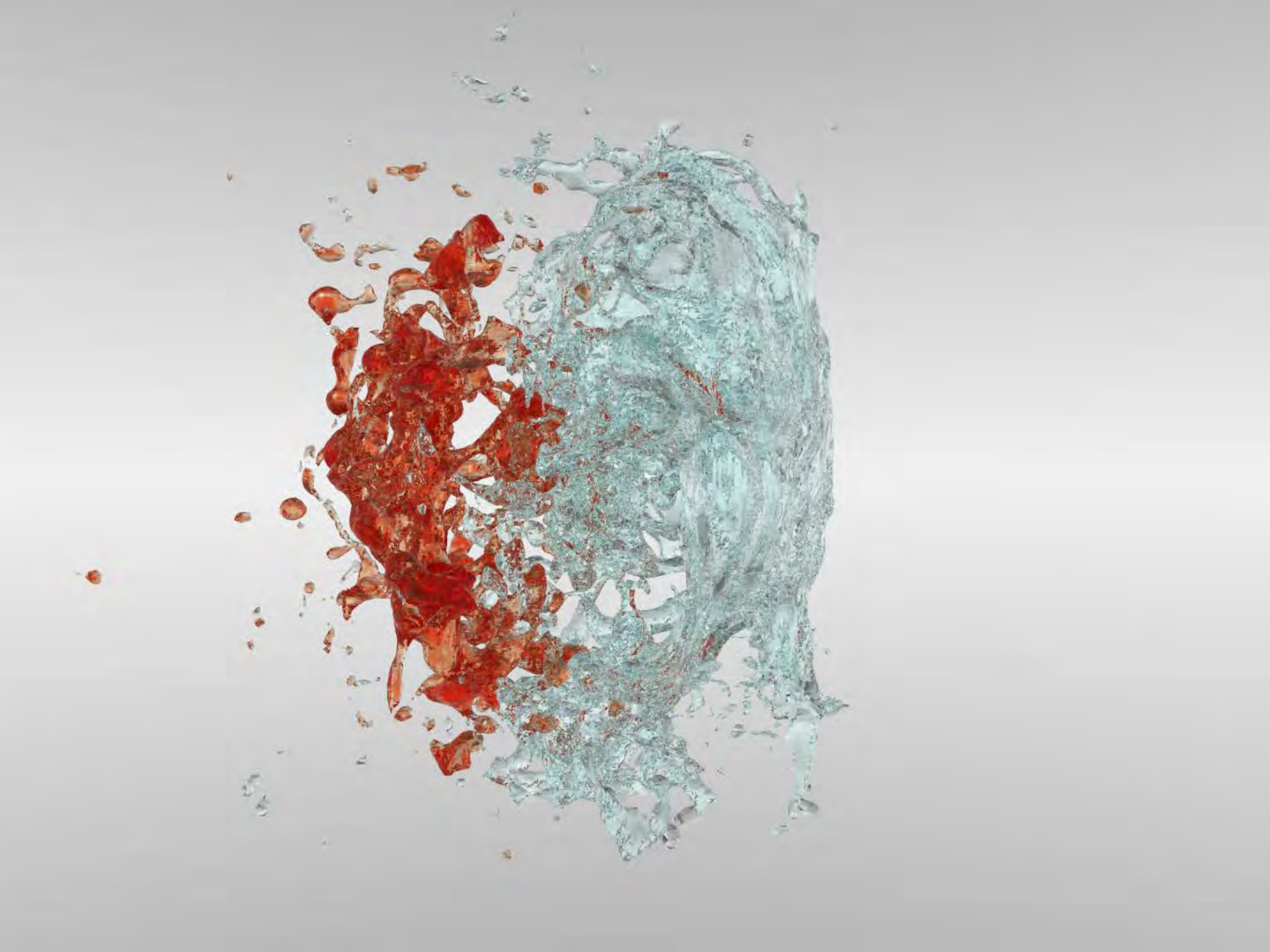








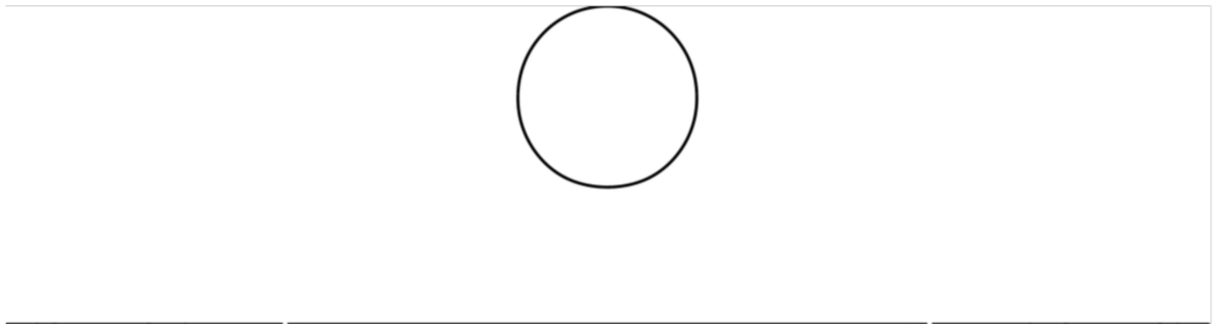


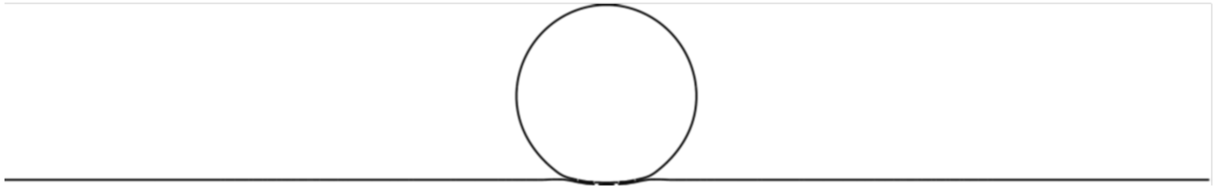


Droplet in Pool with Interfacial Reaction

Axi-symmetric Simulation

School of Aerospace Engineering

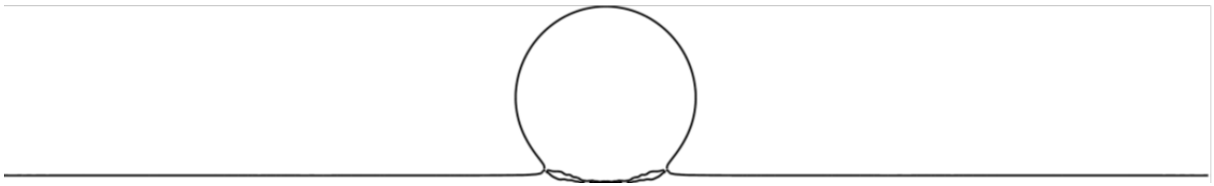


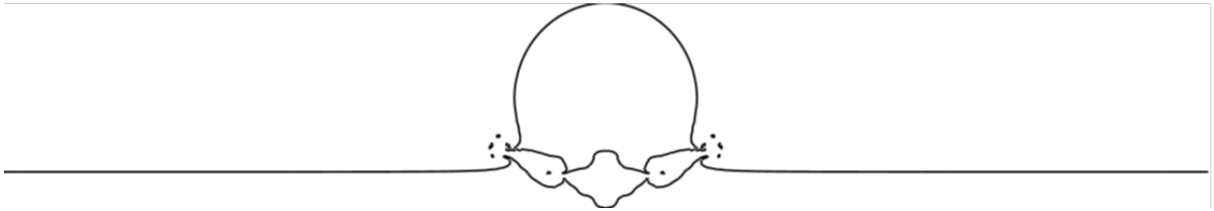


Droplet in Pool with Interfacial Reaction

Axi-symmetric Simulation

School of Aerospace Engineering





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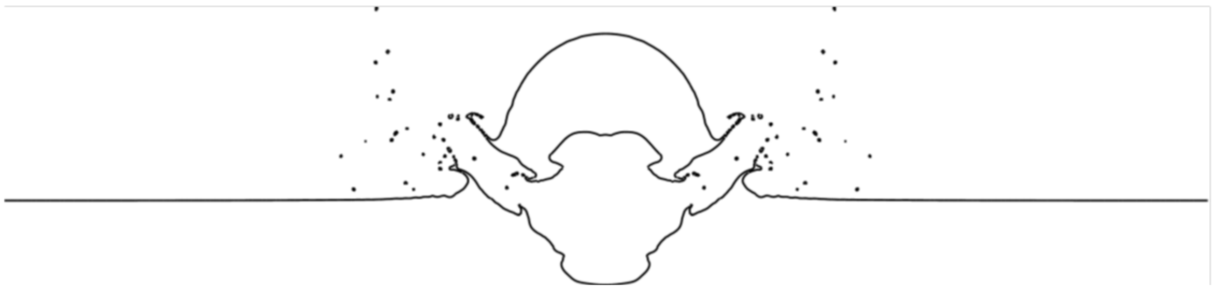
Axi-symmetric Simulation



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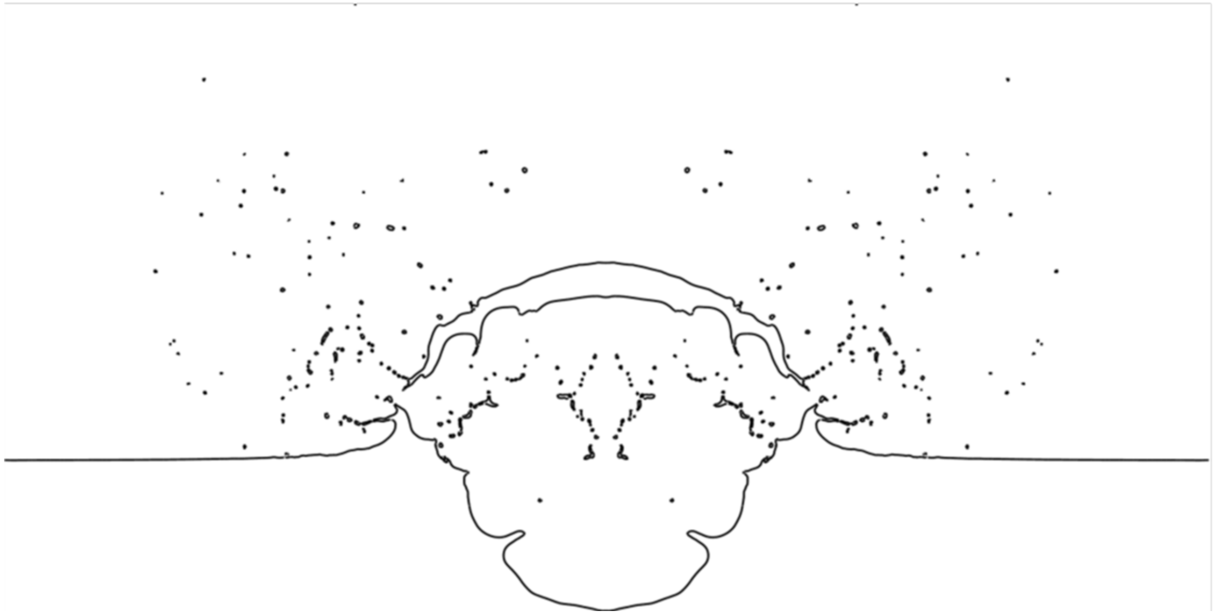
Axi-symmetric Simulation



Droplet in Pool with Interfacial Reaction

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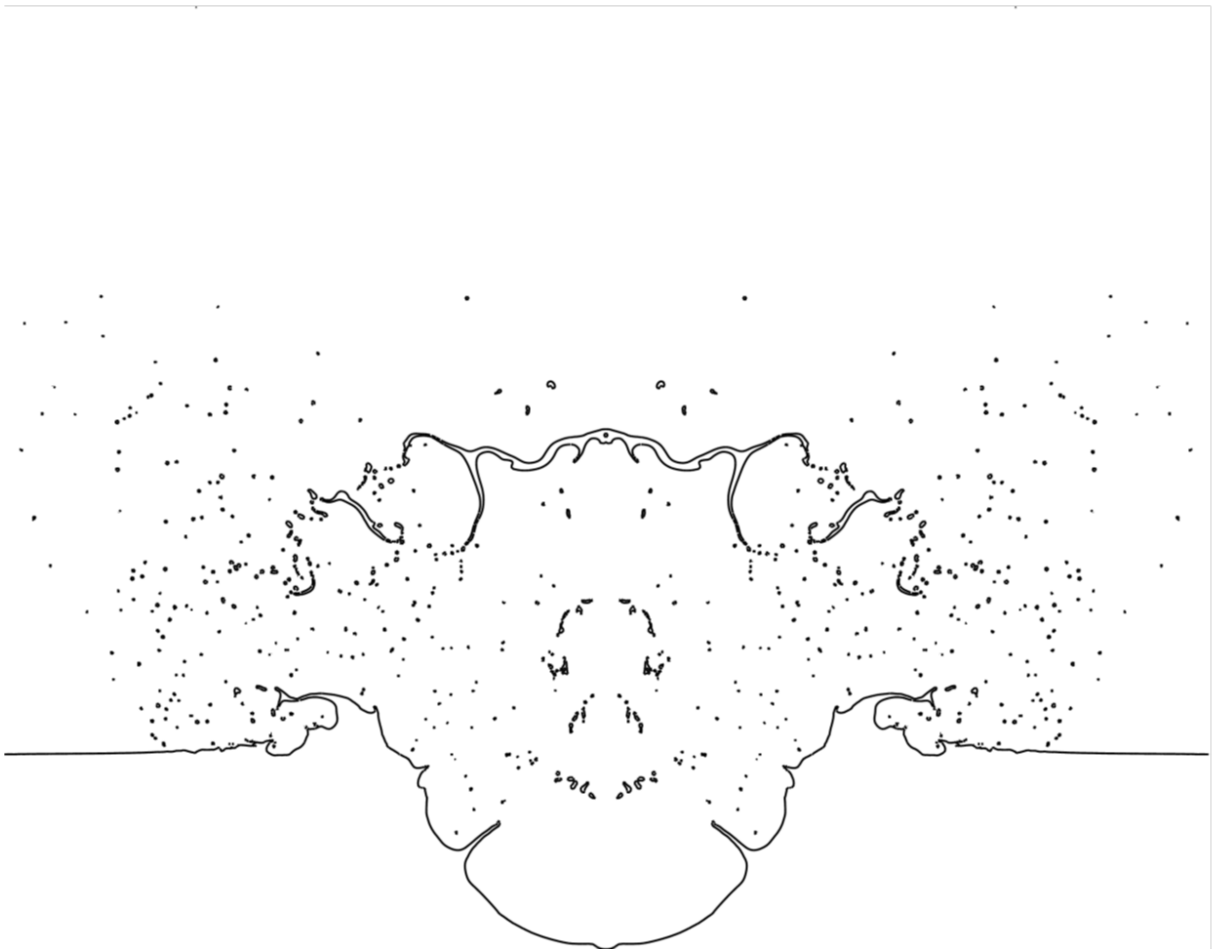

Droplet in Pool with Interfacial Reaction

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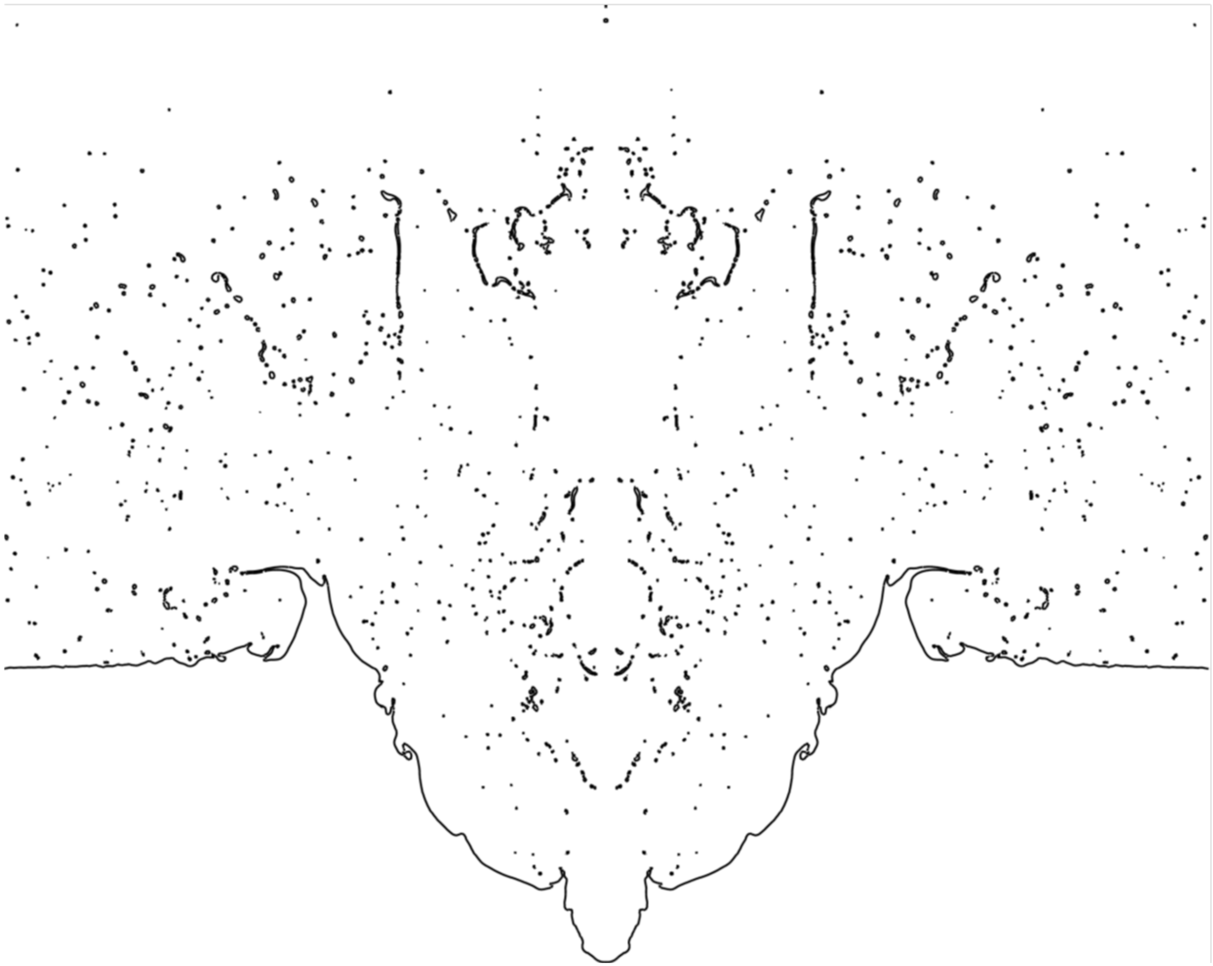
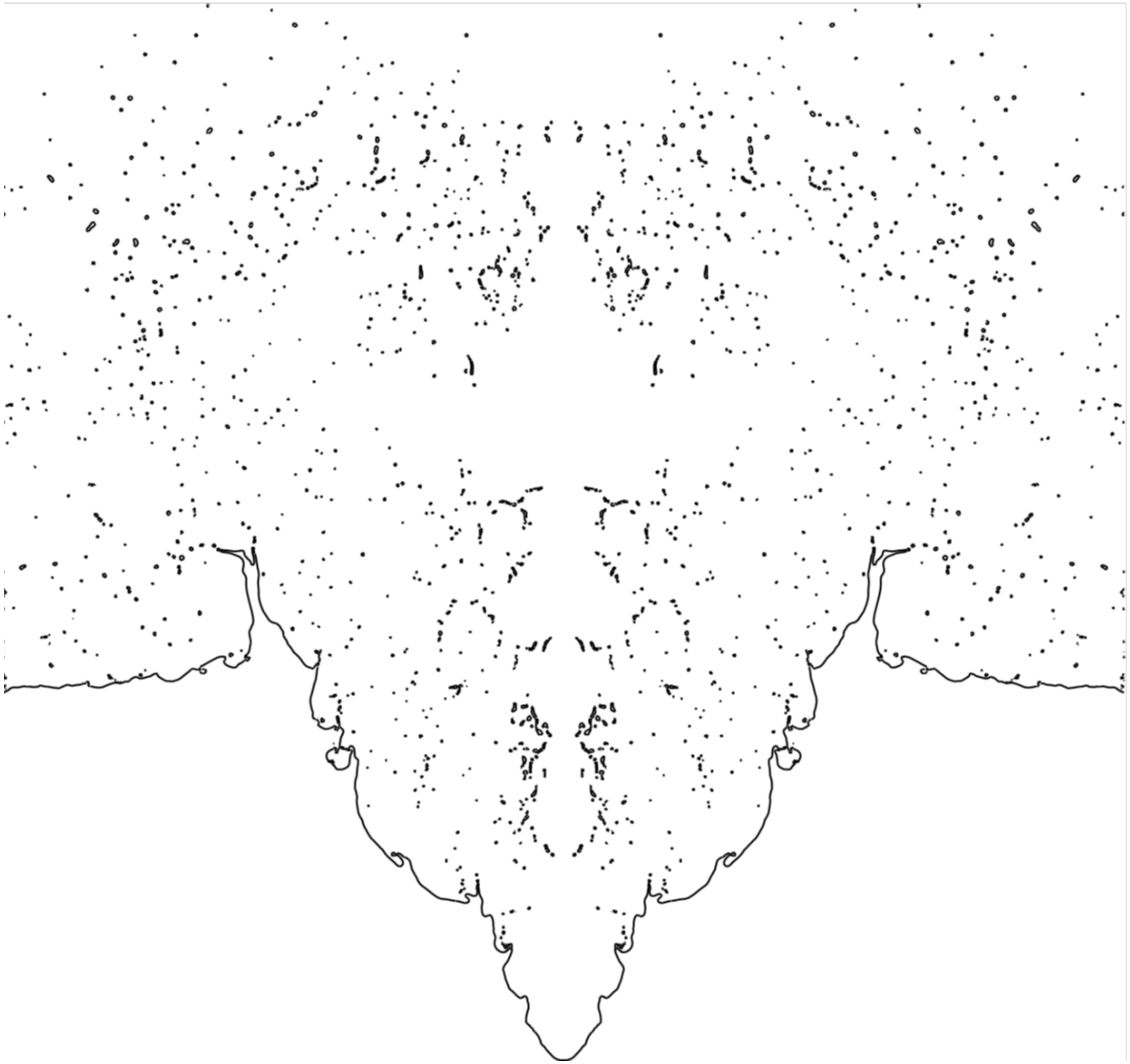


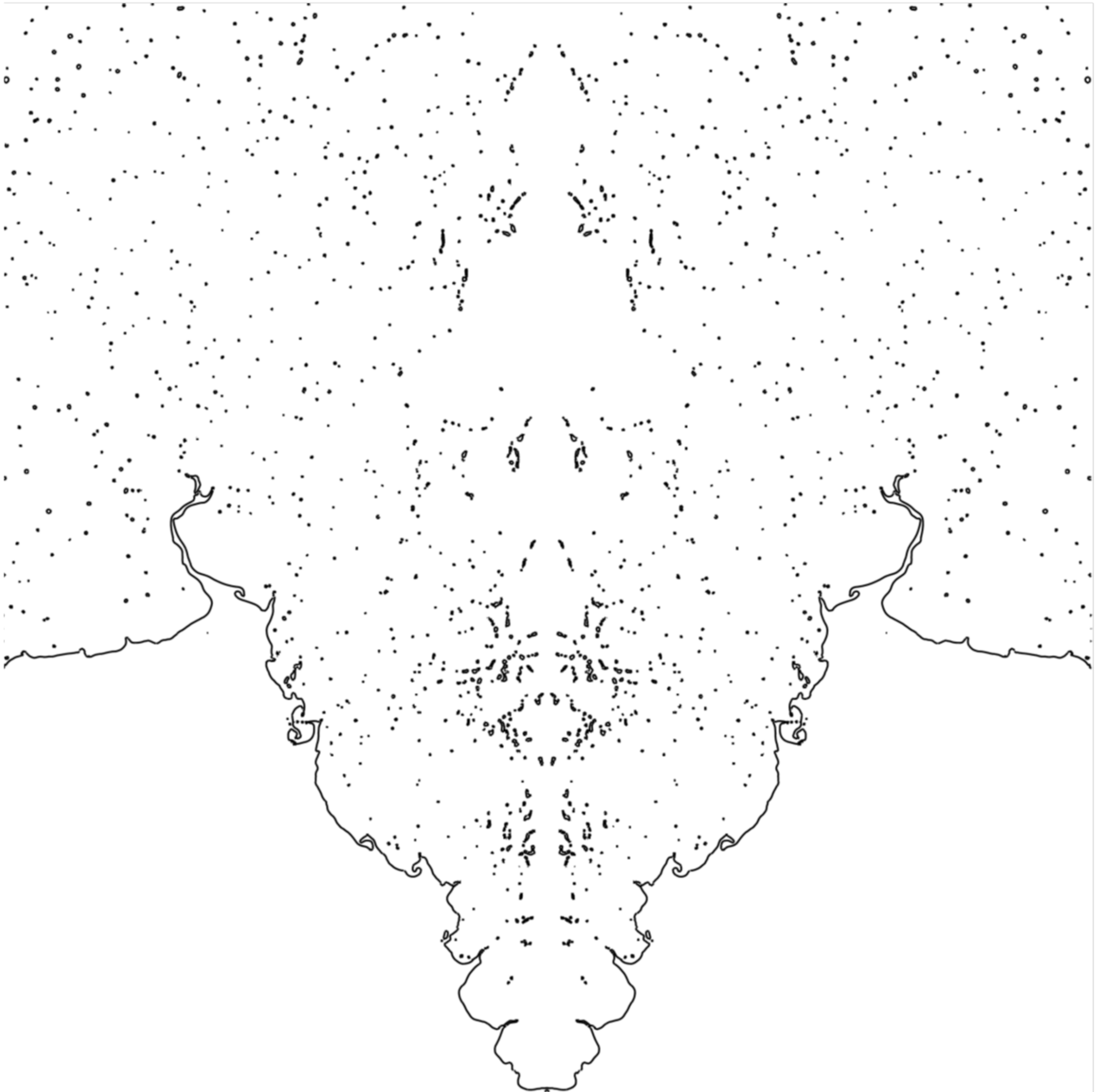
Droplet in Pool with Interfacial Reaction

Axi-symmetric Simulation



Droplet in Pool with Interfacial Reaction

Axi-symmetric Simulation



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Droplet in Pool with Interfacial Reaction

Axi-symmetric Simulation

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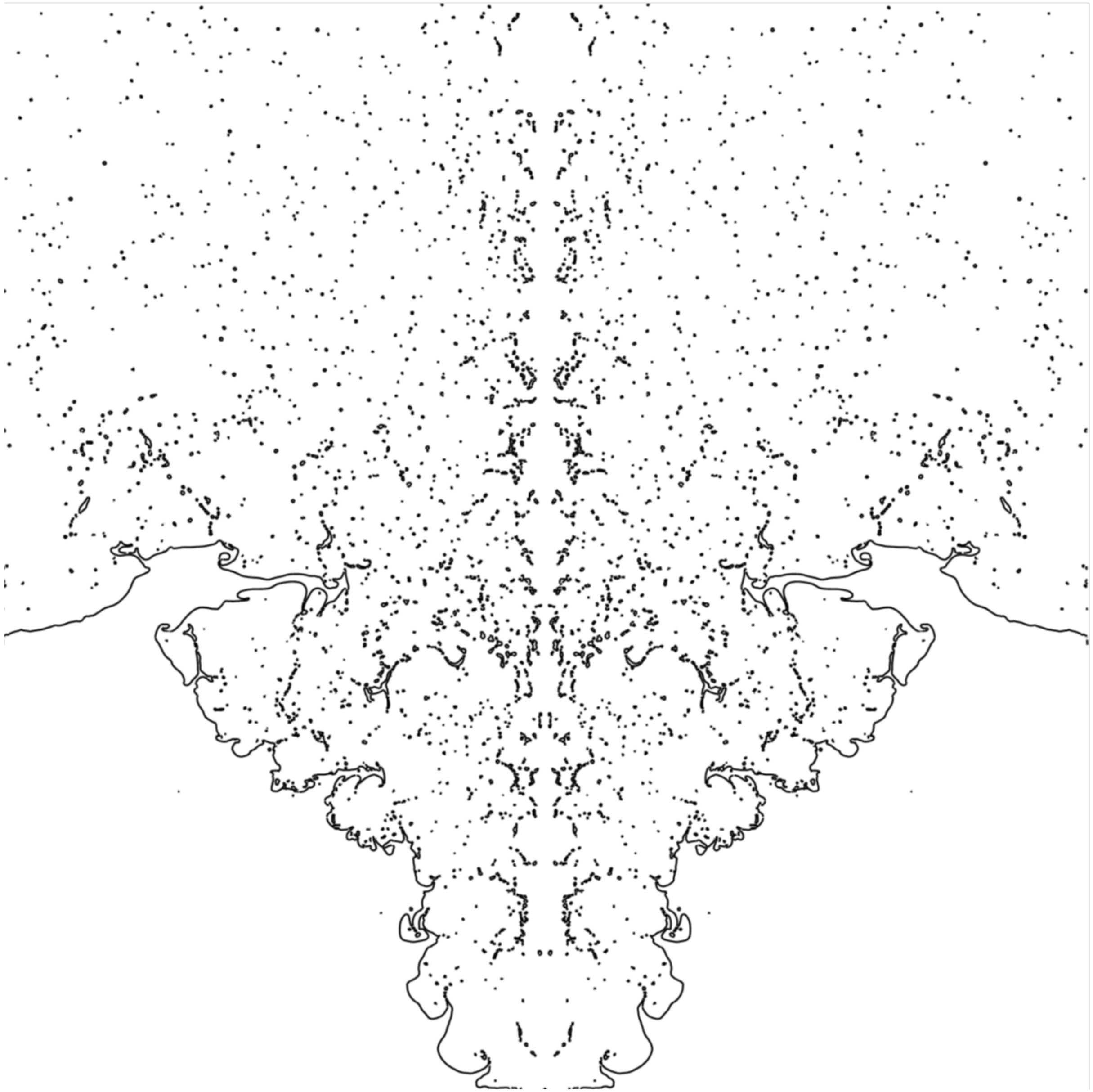
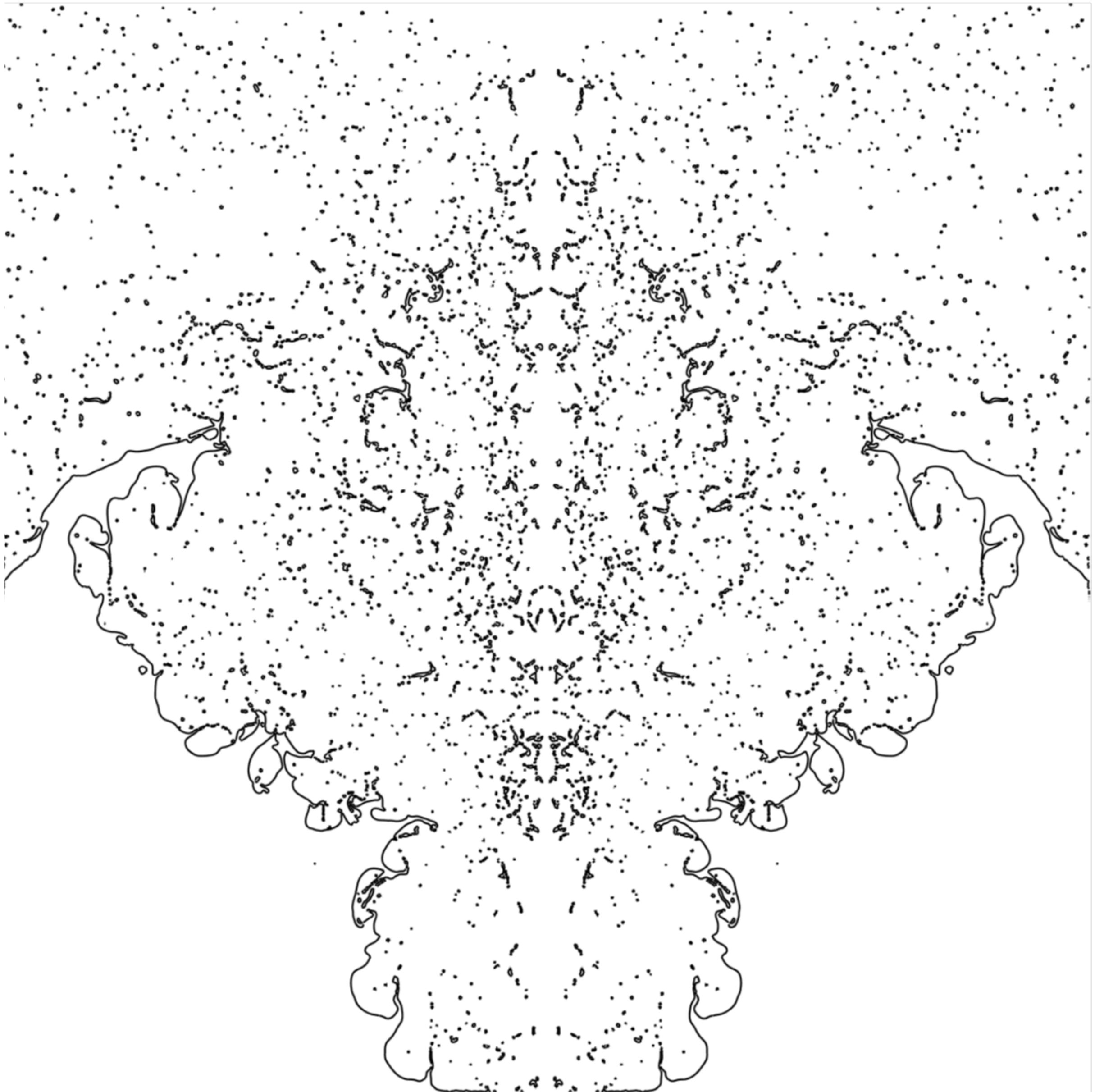


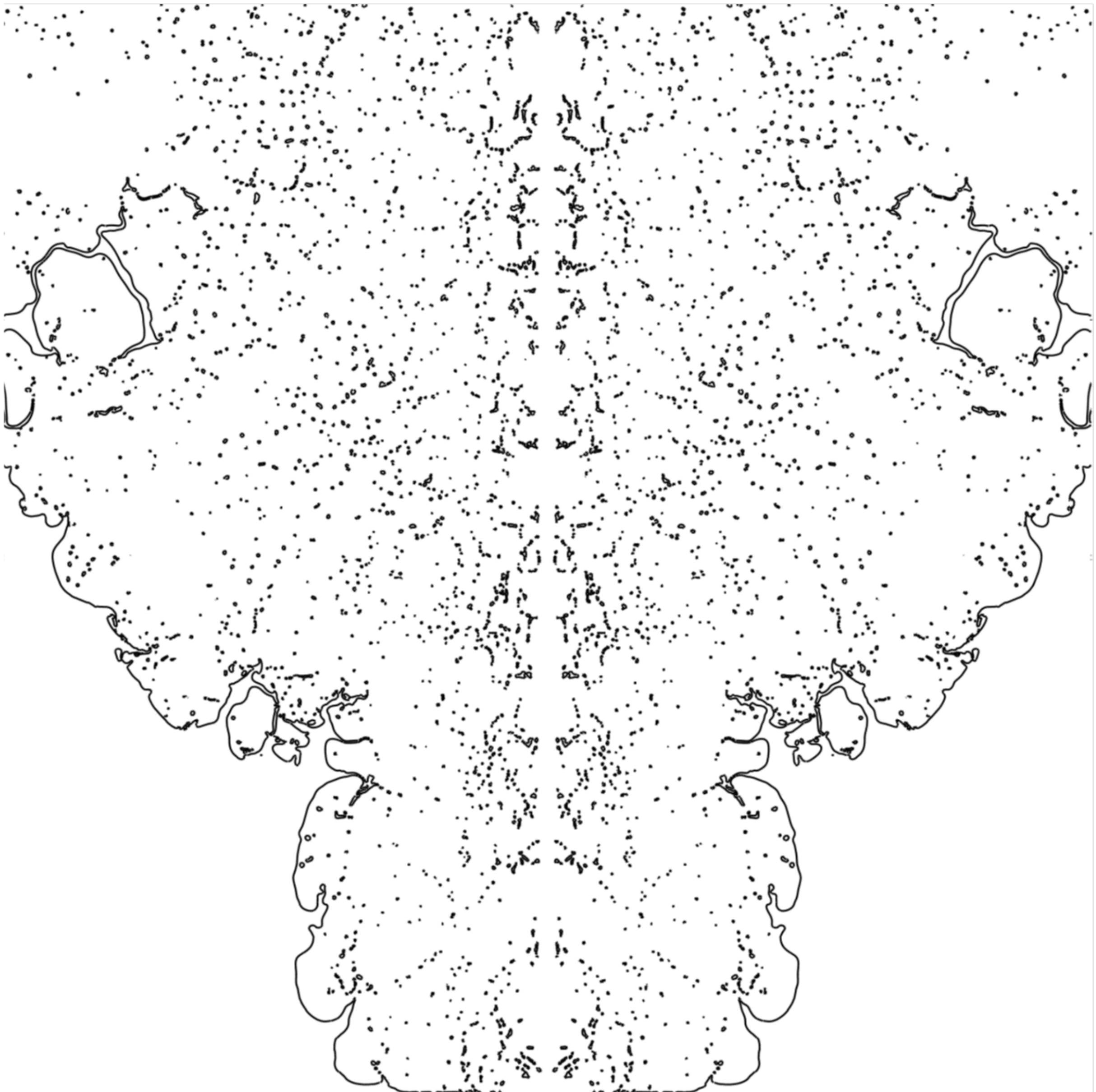
Droplet in Pool with Interfacial Reaction

Axi-symmetric Simulation



Droplet in Pool with Interfacial Reaction

Axi-symmetric Simulation



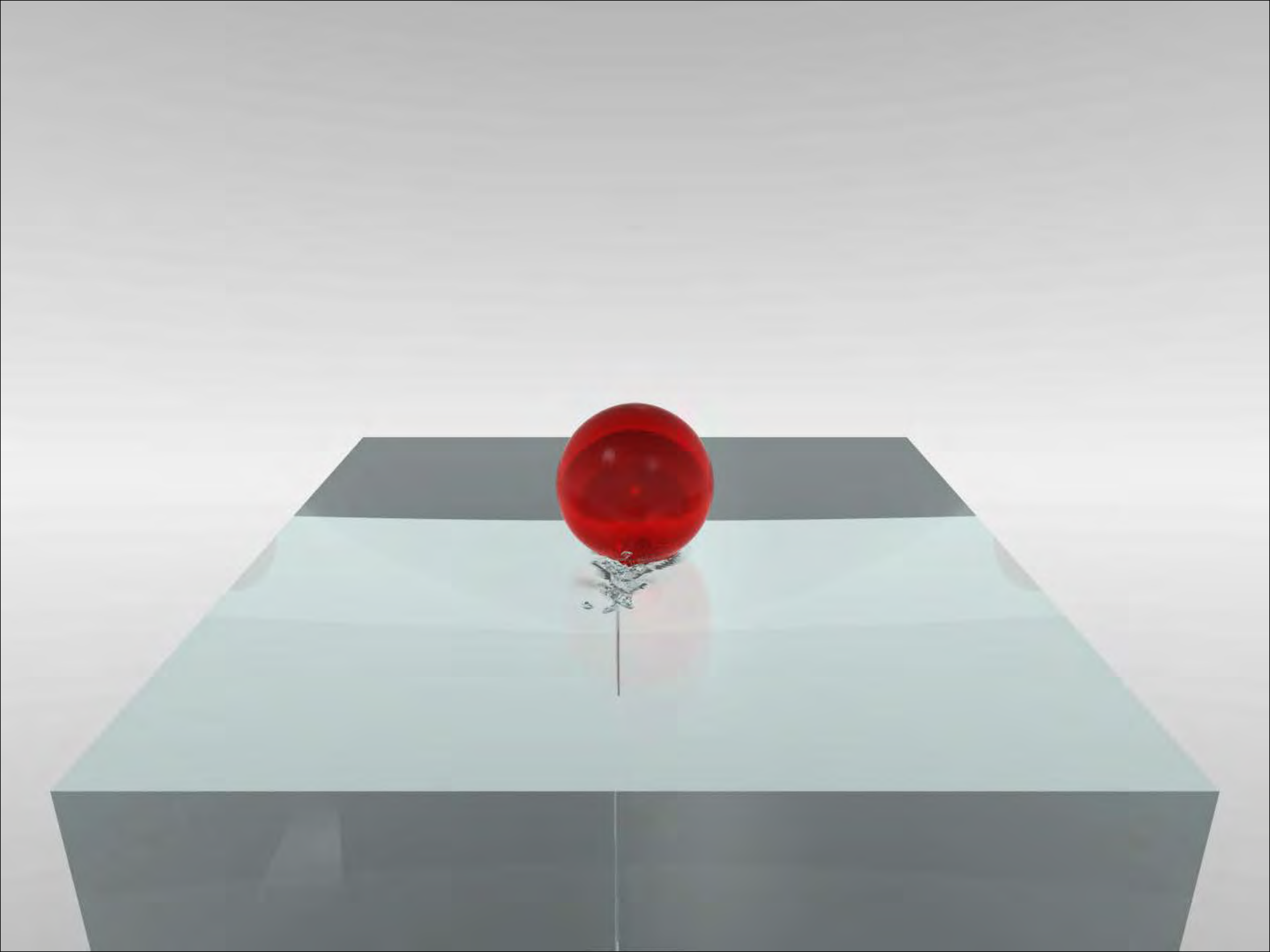
Droplet in Pool with Interfacial Reaction

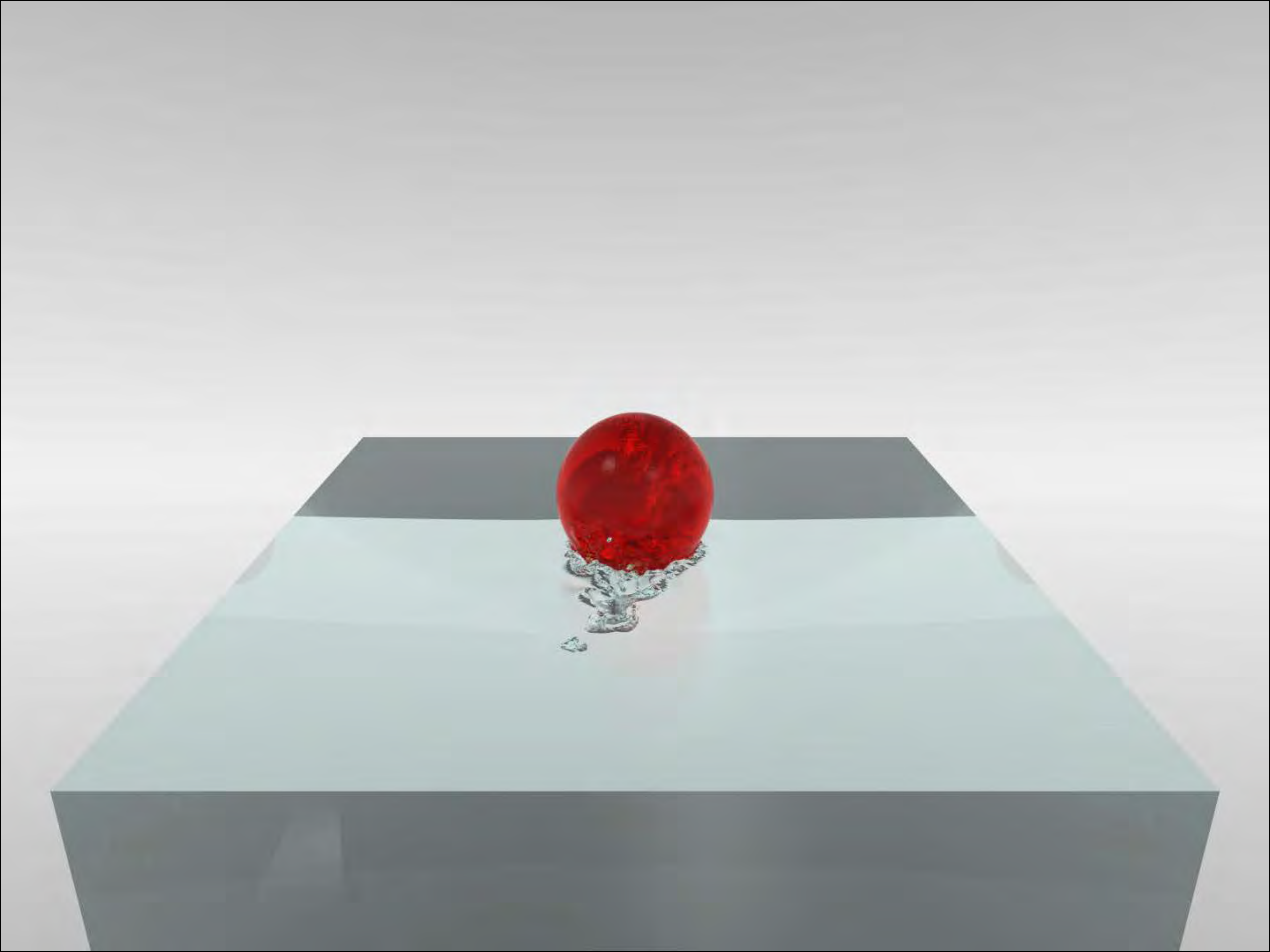
Axi-symmetric Simulation

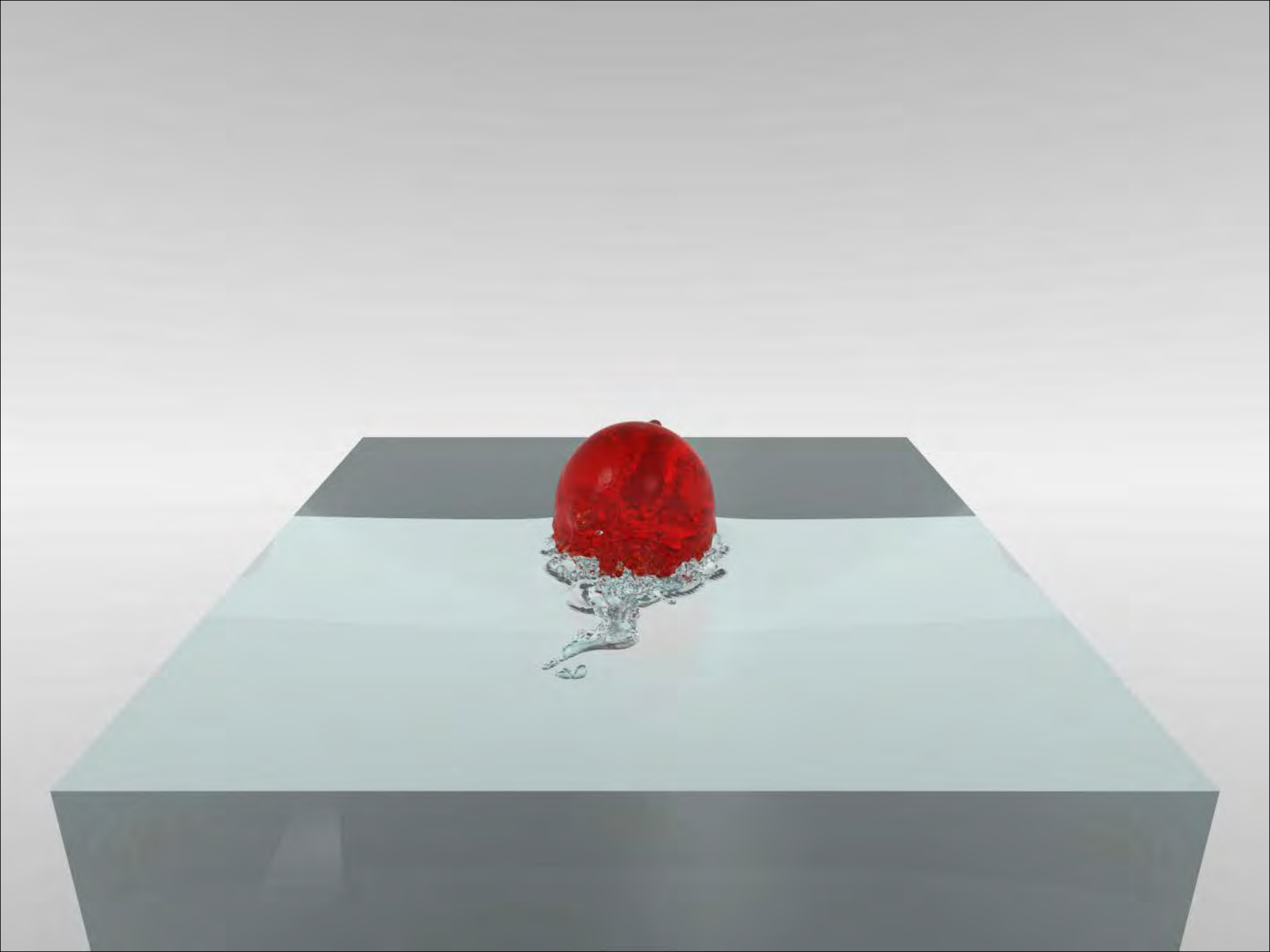
Droplet in Pool with Interfacial Reaction

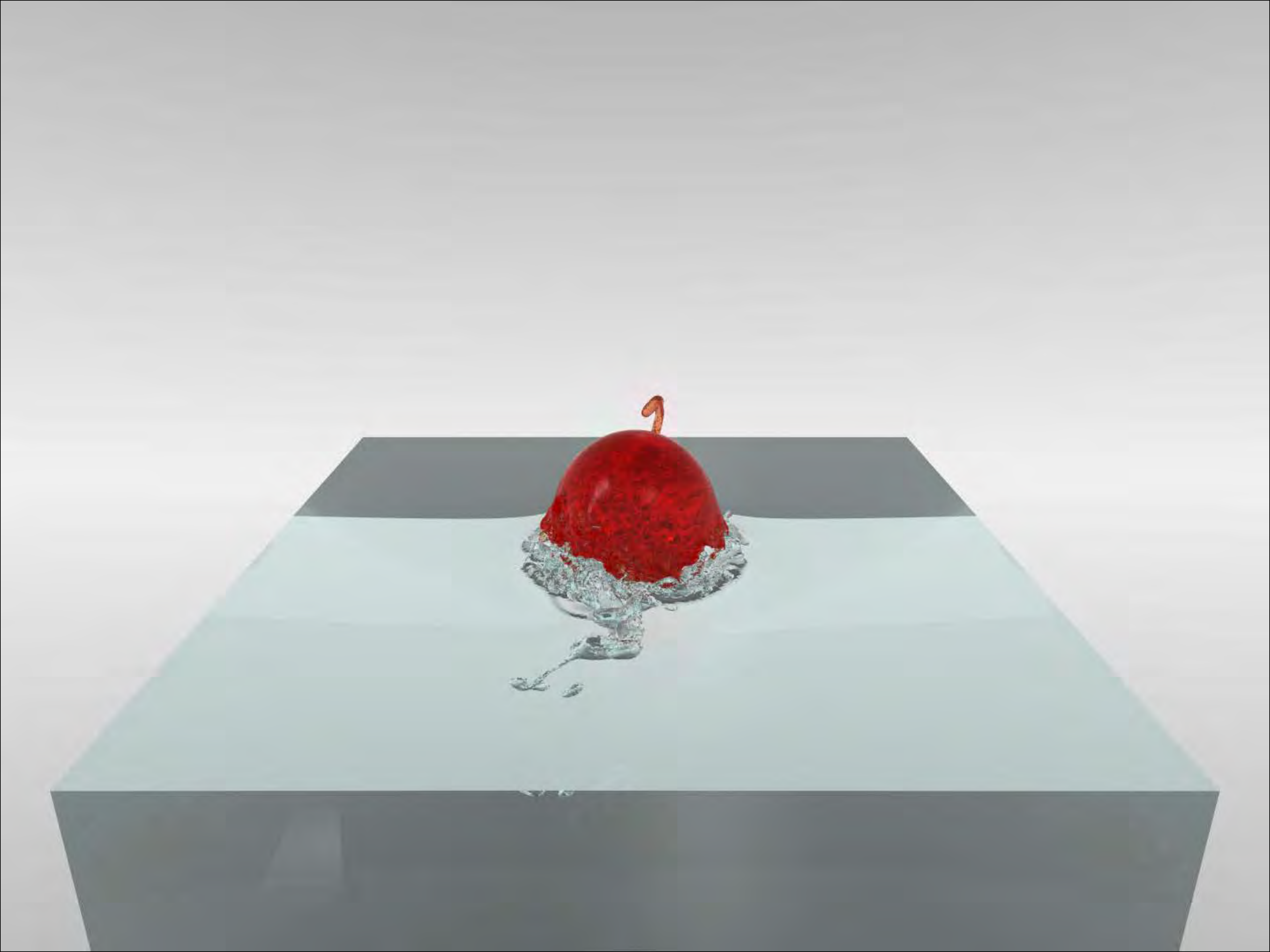
3-D simulation

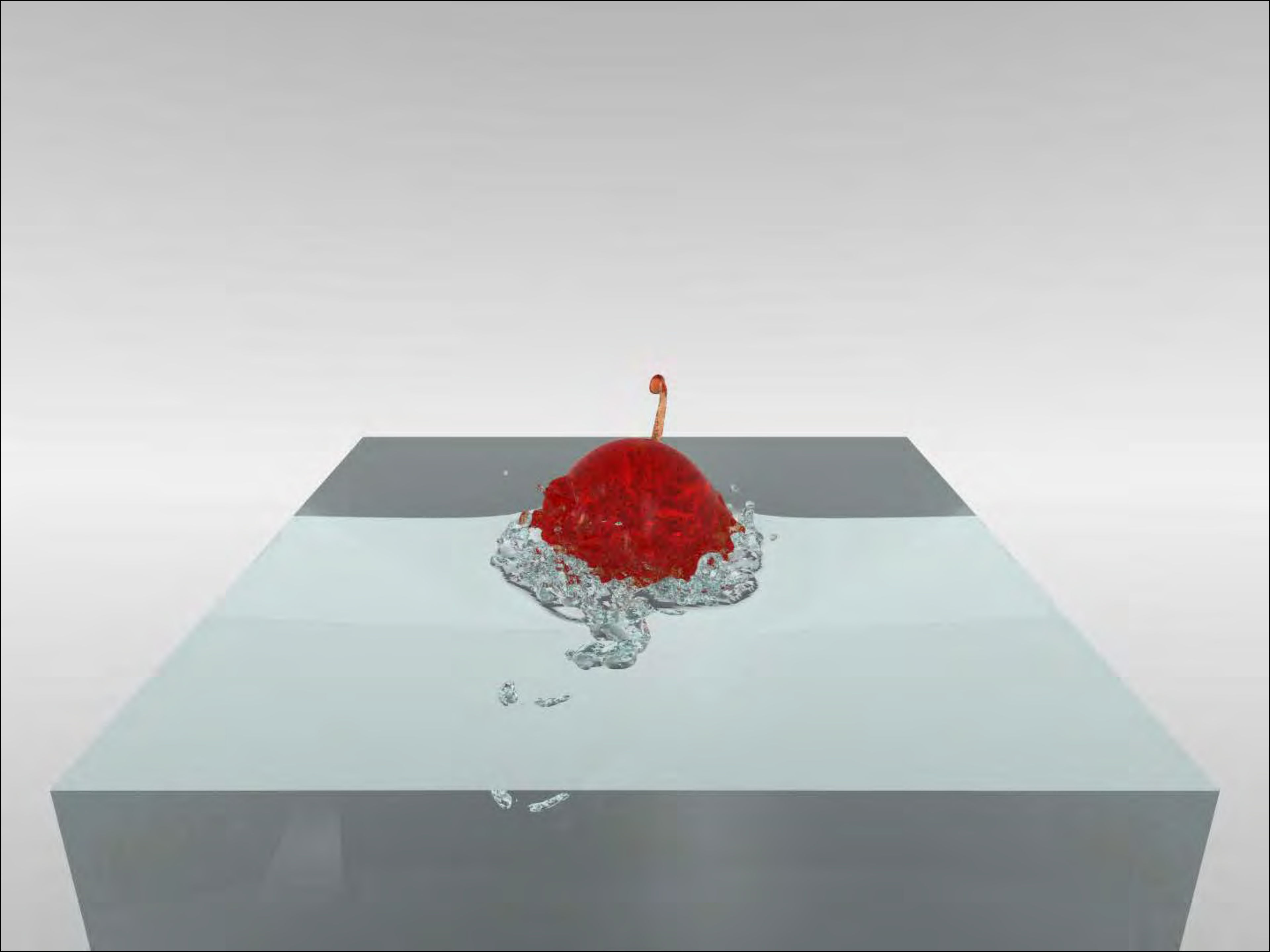
Movie

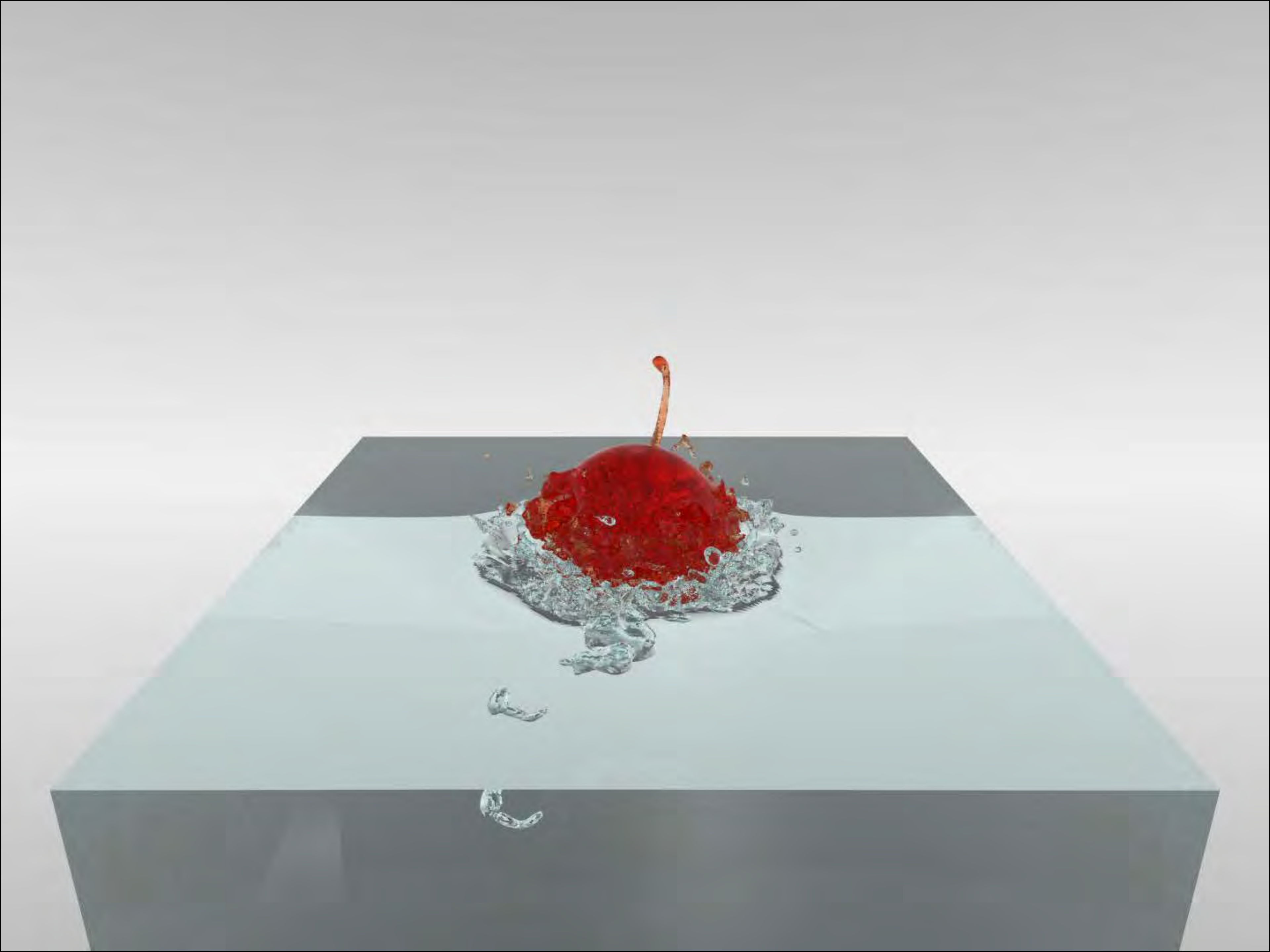


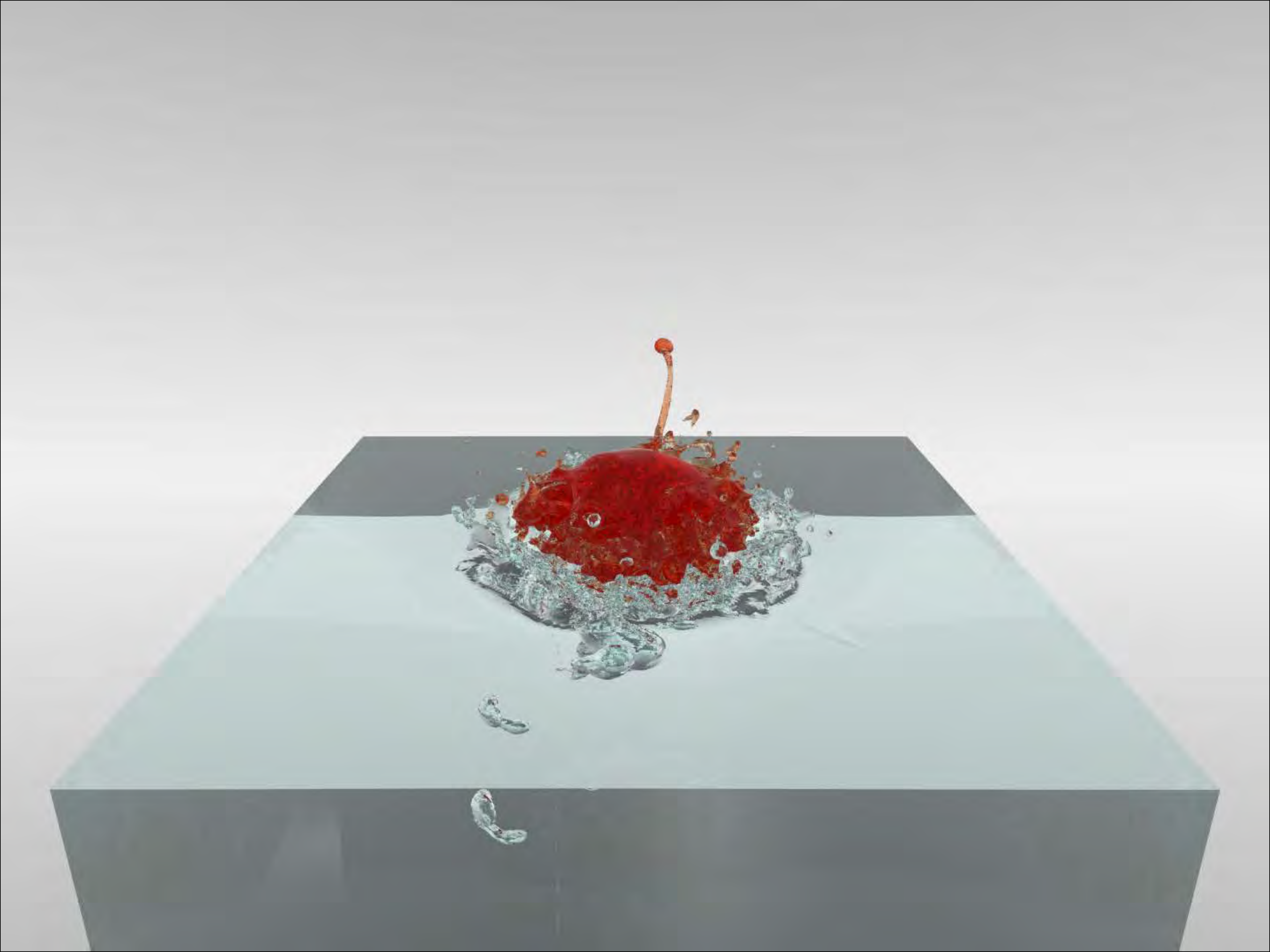


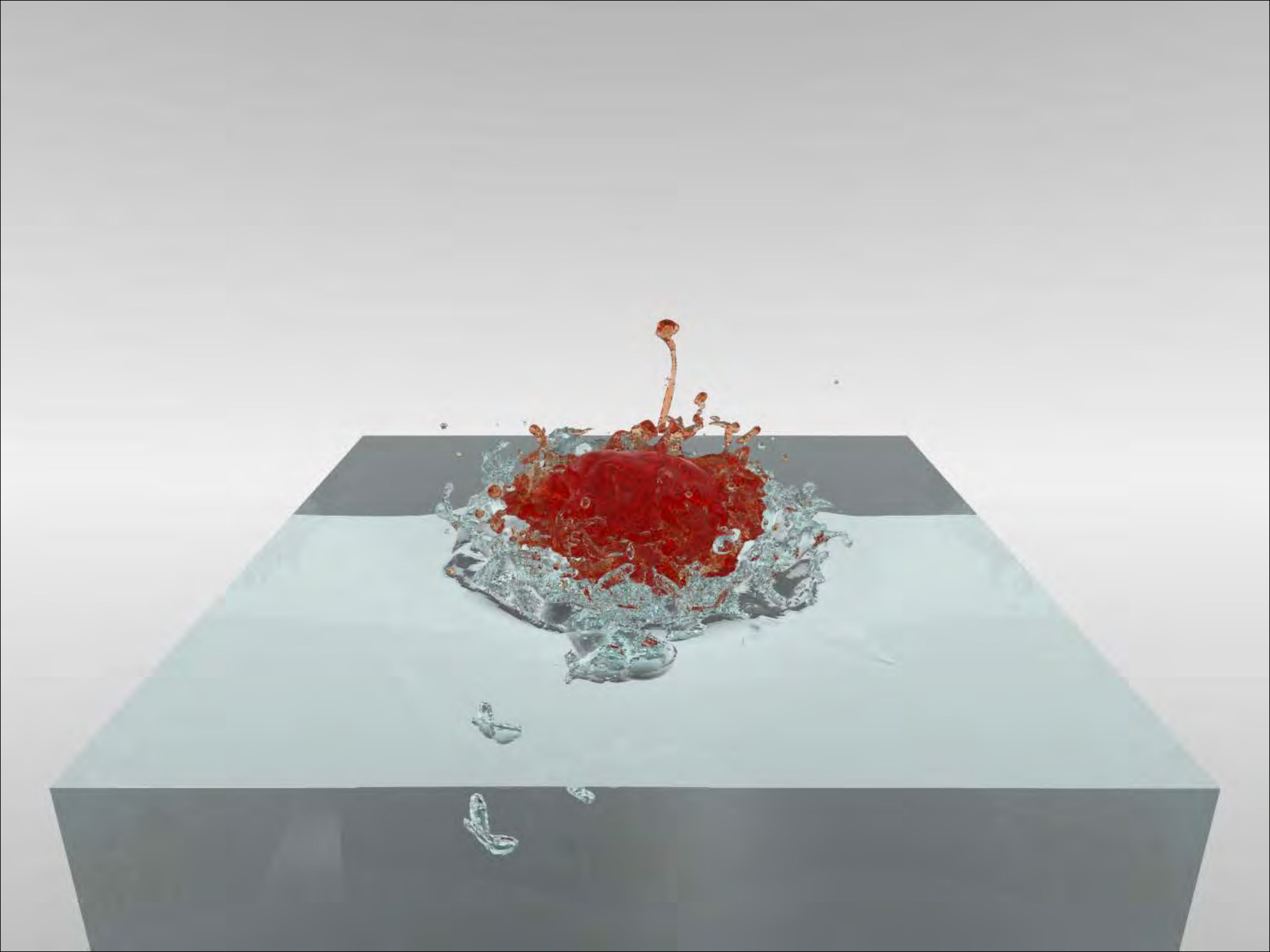


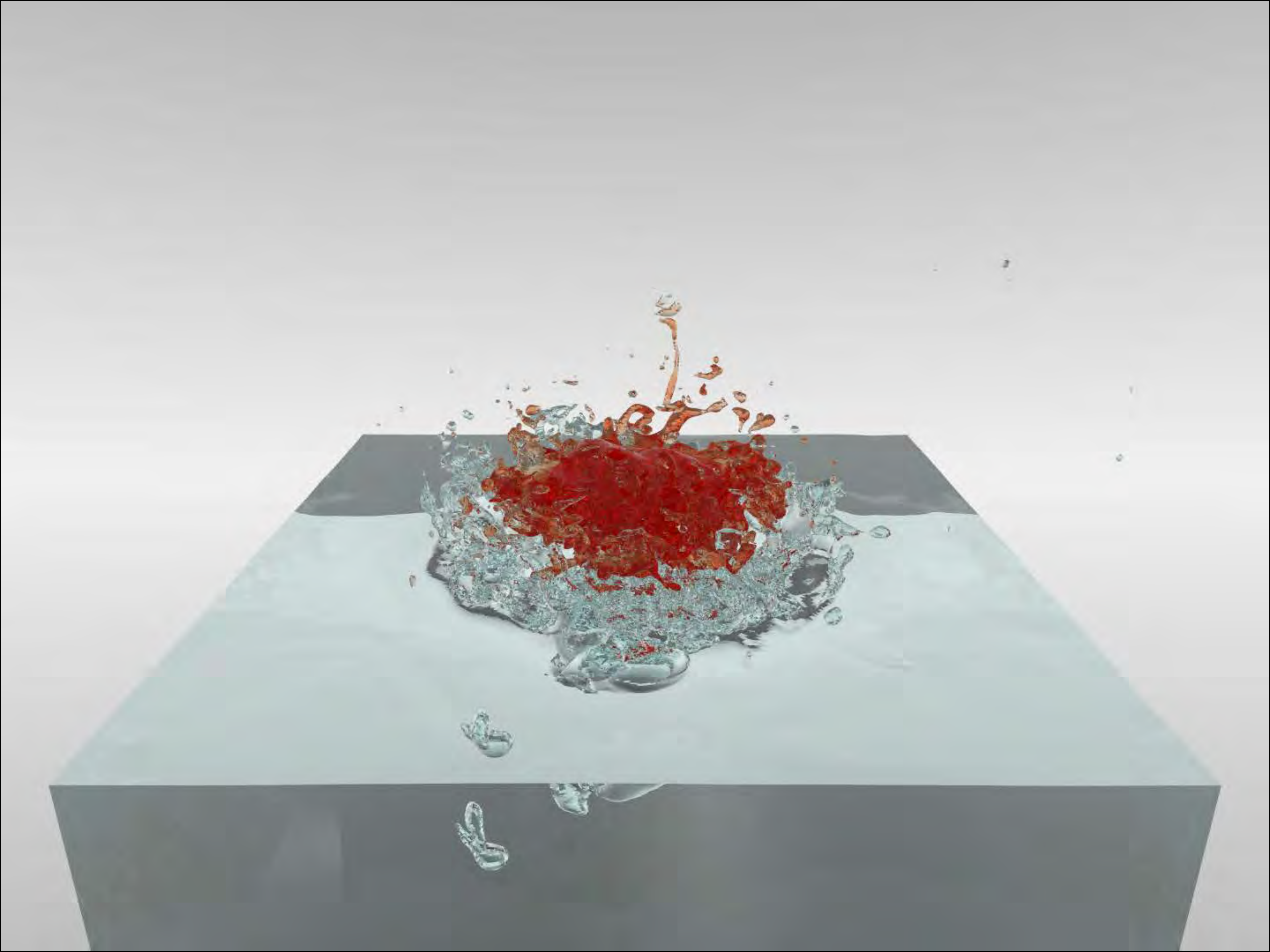


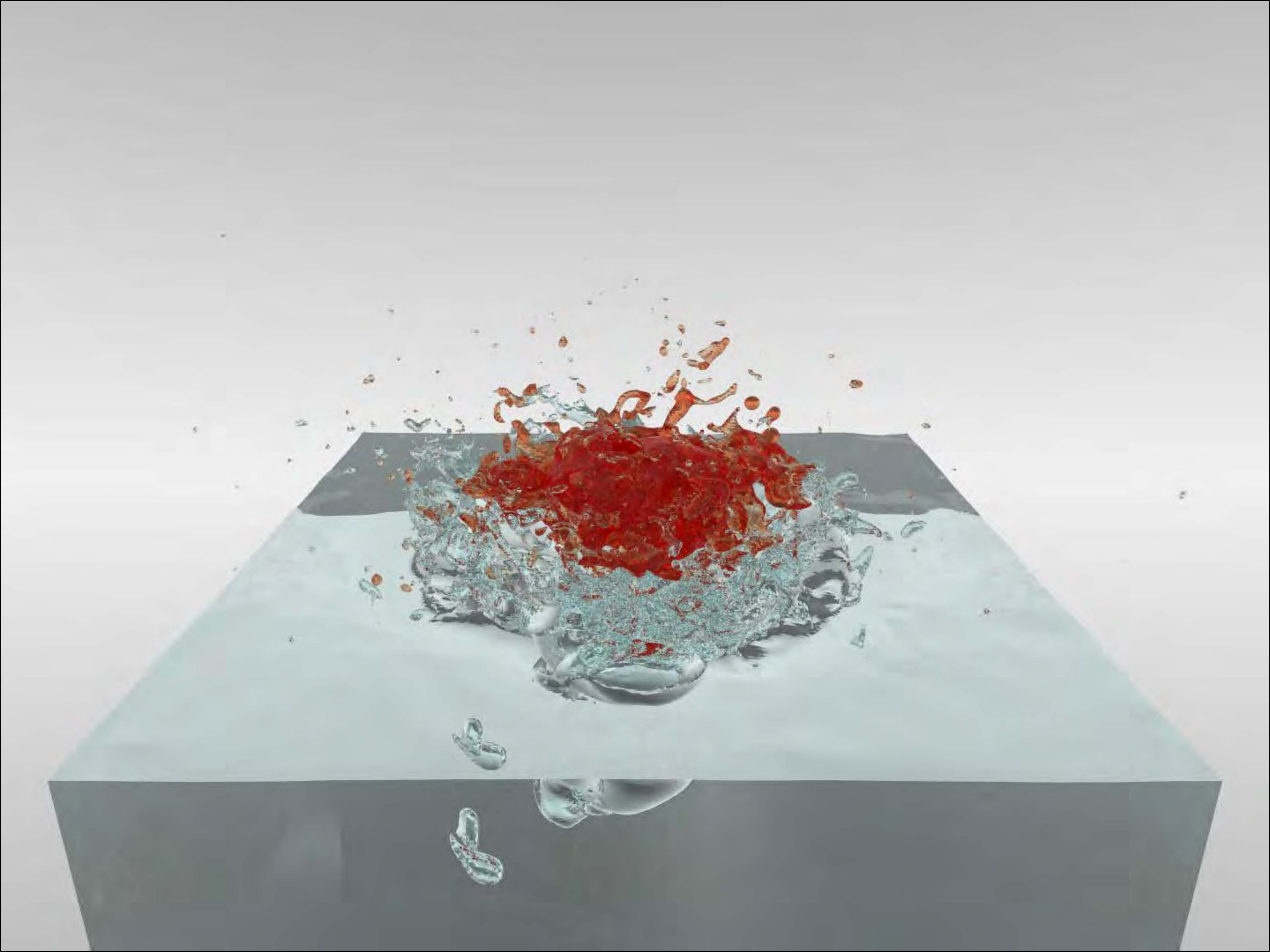


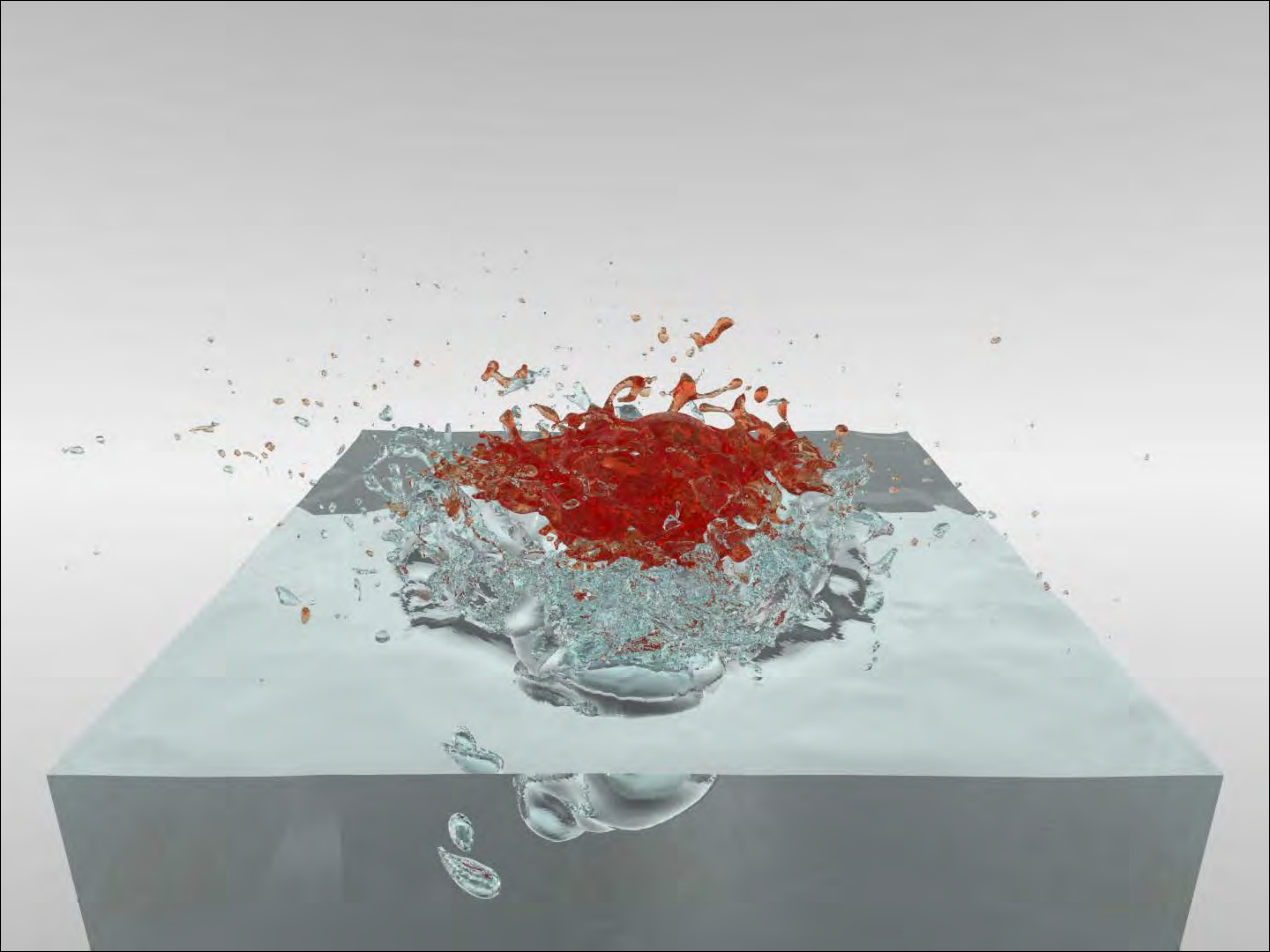


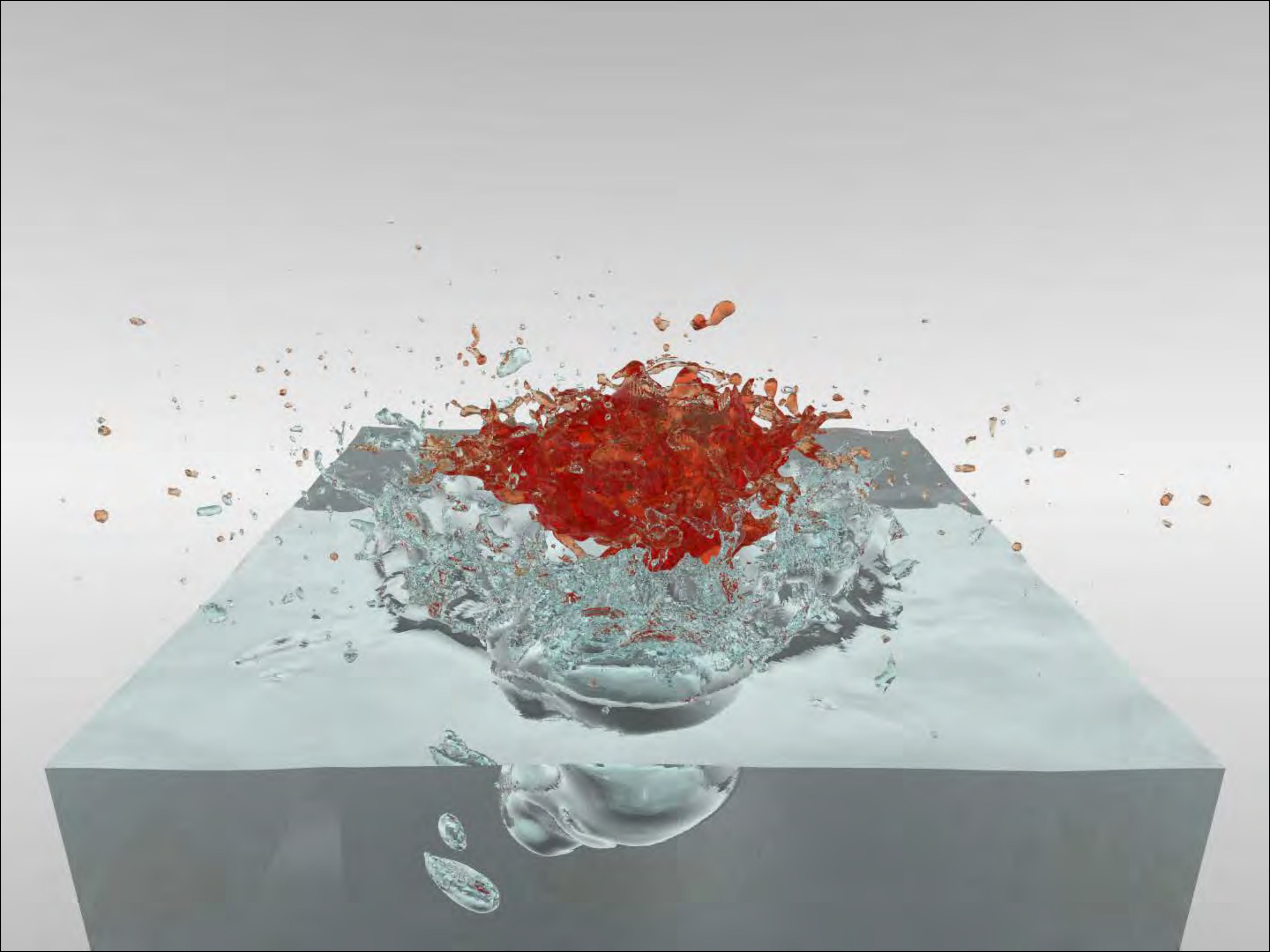


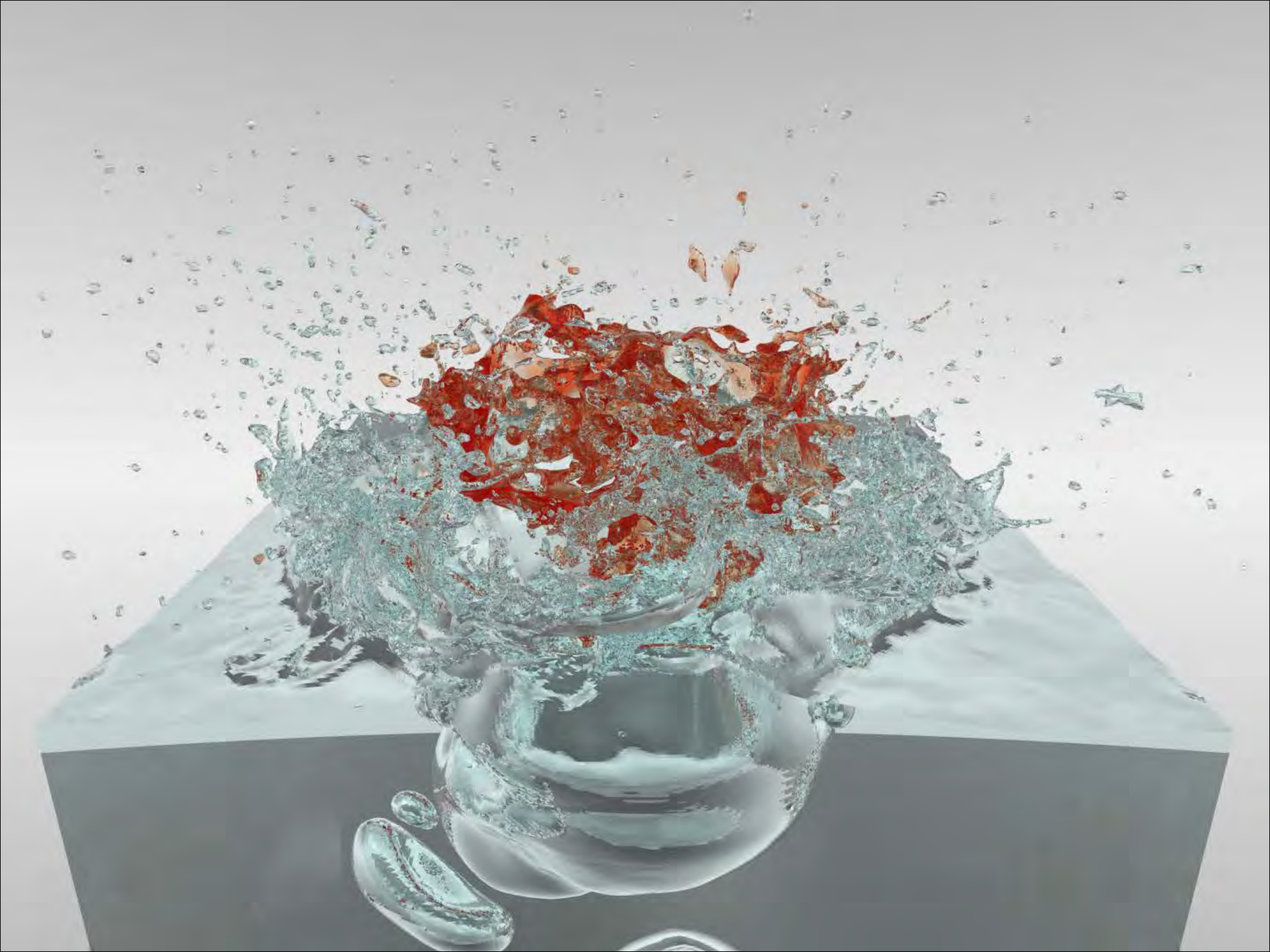












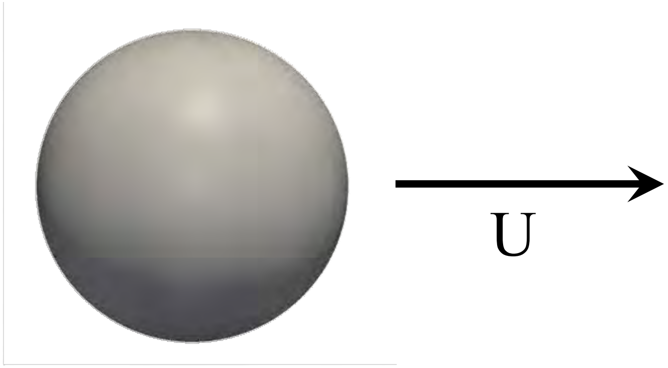
Breakup of Liquid Droplets

Dimensional Analysis

$$f(t, u, D, \sigma, \mu_g, \mu_l, \rho_g, \rho_l) = 0$$

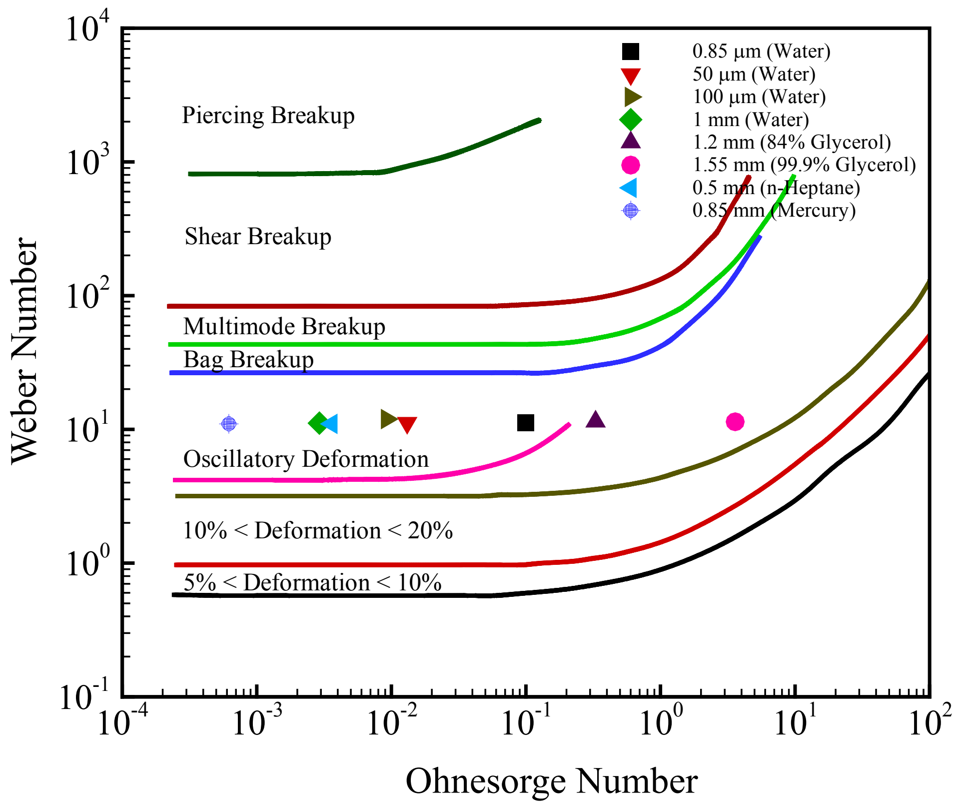
$$F(\pi_1, \pi_2, \pi_3, \pi_4, \pi_5) = 0$$

Weber number, *We*	$\dfrac{\rho_g U^2 D}{\sigma}$
Reynolds number, *Re*	$\dfrac{\rho_g U D}{\mu_g}$
Density ratio	$\dfrac{\rho_l}{\rho_g}$
Viscosity ratio	$\dfrac{\mu_l}{\mu_g}$
Ohnesorge number, *Oh*	$\dfrac{\mu_l}{\sqrt{\rho_l D \sigma}}$



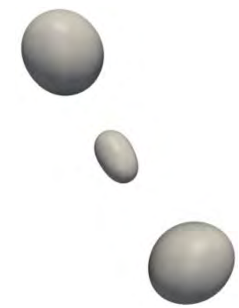
Time Scale	Definition	Remarks
convective time	$\tau_c = D/U$	
deformation response time	$\tau_r = \sqrt{\rho_l D^3/\sigma}$	$\tau_r^2 = We \dfrac{\rho_l}{\rho_g} \tau_c^2$
transport time (gas)	$\tau_{v,g} = D^2/\nu_g$	$\tau_r^2 = \dfrac{We}{\mathrm{Re}^2} \dfrac{\rho_l}{\rho_g} \tau_{v,g}^2$
transport time (liquid)	$\tau_{v,l} = D^2/\nu_l$	$\tau_r^2 = \dfrac{We}{\mathrm{Re}^2} \dfrac{\rho_l}{\rho_g} \dfrac{\nu_l^2}{\nu_g^2} \tau_{v,l}^2$

Breakup Regime Diagram (1 atm)



$$Oh = \frac{\mu_l}{\sqrt{\rho_l D \sigma}} \qquad We = \frac{\rho_g U^2 D}{\sigma}$$

Oscillatory breakup



Bag breakup

Multimode breakup

Shear breakup

Fluid (in air)	ρ (kg/m³)	μx10⁴ (kg/m-s)	σx10³ (N/m)
Water	1000	7.89	72.8
n-Heptane	683	3.94	20.0
Mercury	13600	15.0	475.0
Glycerol (84%)	1219	1000	63.2
Glycerol (99.9%)	1260	12500	62.0

L.-P. Hsiang & G. M. Faeth, Drop deformation and breakup due to shock wave and steady disturbances, IJMF, 1995.

Georgia Tech

Breakup Regime Diagram (1 atm)

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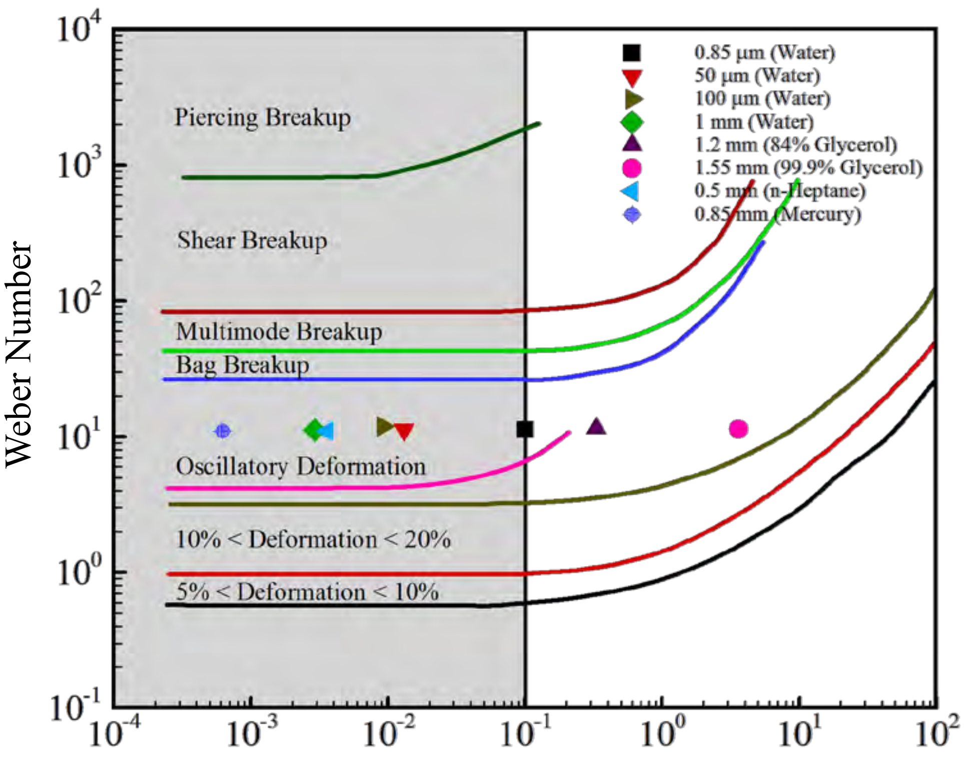
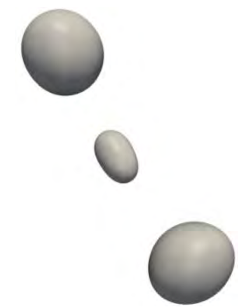


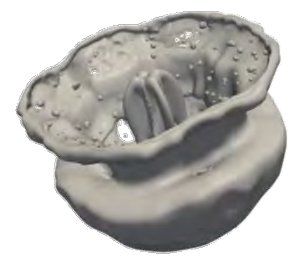
$$Oh = \frac{\mu_l}{\sqrt{\rho_l D \sigma}} \qquad We = \frac{\rho_g U^2 D}{\sigma}$$

Oscillatory breakup



Bag breakup

Multimode breakup



Shear breakup

Fluid (in air)	ρ (kg/m^3)	μx10^4 (kg/m-s)	σx10^3 (N/m)
Water	1000	7.89	72.8
n-Heptane	683	3.94	20.0
Mercury	13600	15.0	475.0
Glycerol (84%)	1219	1000	63.2
Glycerol (99.9%)	1260	12500	62.0

L.-P. Hsiang & G. M. Faeth, Drop deformation and breakup due to shock wave and steady disturbances, IJMF, 1995.

Oscillatory Breakup
water droplet in air (100 atm)

School of Aerospace Engineering

Diameter (μm)	Velocity (m/s)	p (atm)	We_g	Re_g
100	12	100	24	7609

t = 4.16 μs

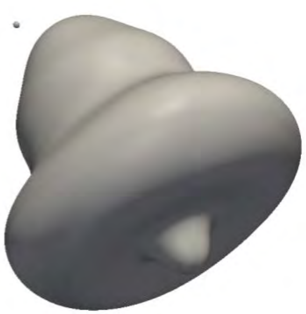
t = 50 μs

t = 66.6 μs

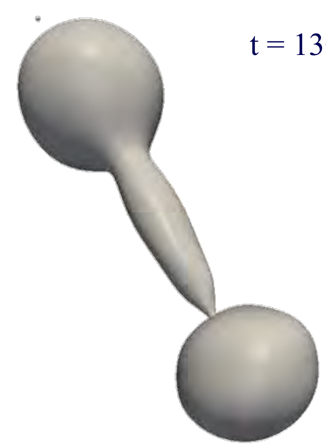
Lateral deformation and bag formation

Oscillation and dome formation

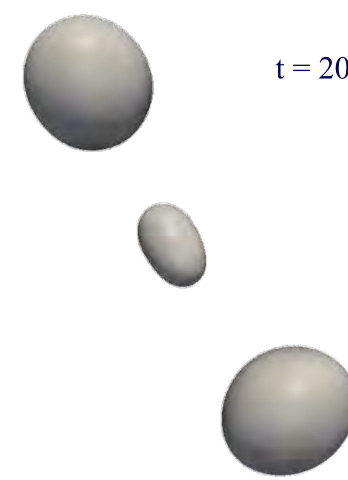
t = 83.3 μs



t = 130 μs



t = 204.6 μs

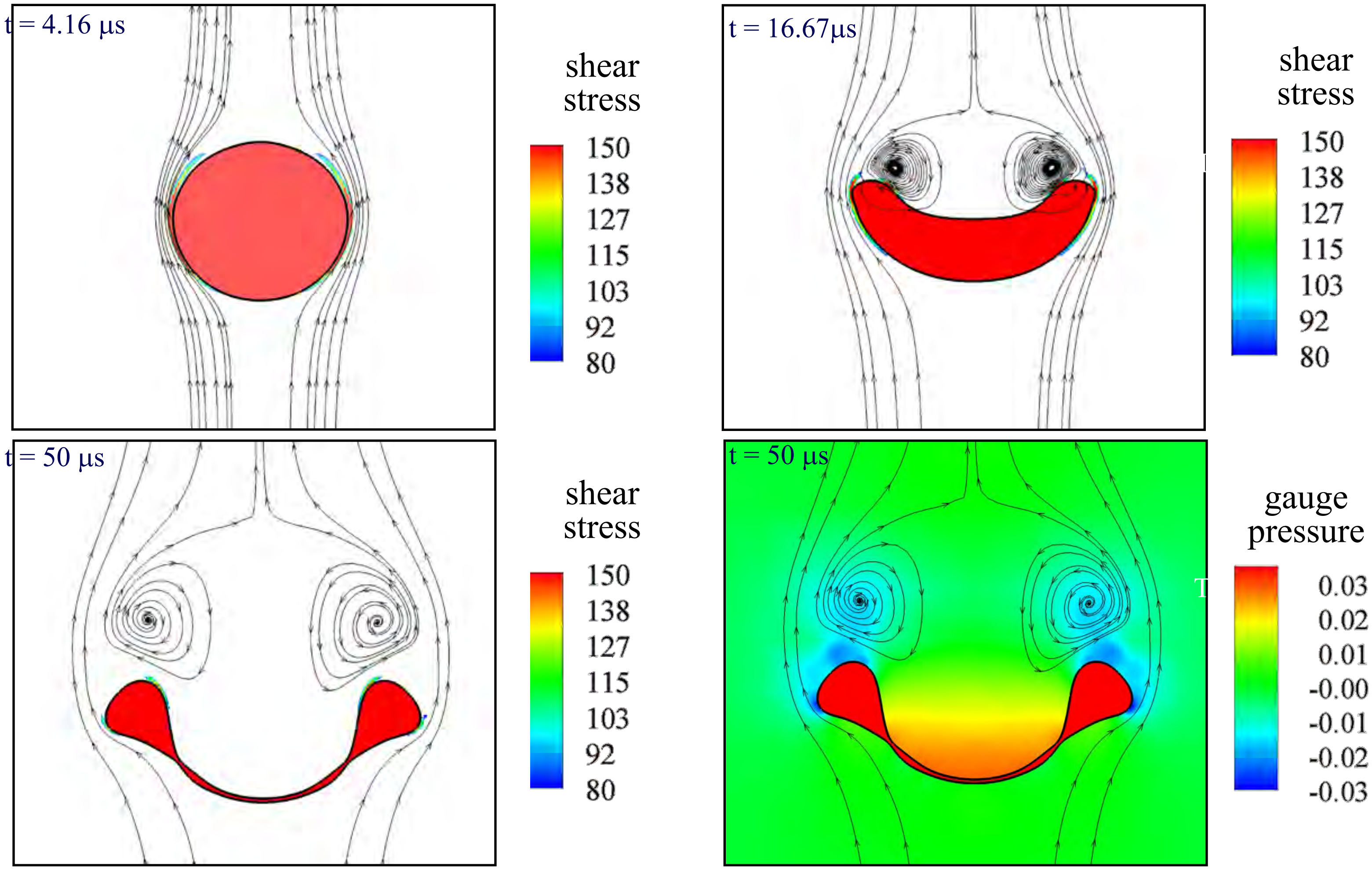


Droplet stretching and breakup

spatial resolution: 10^{-3} droplet diameter

Oscillatory Breakup of Water Droplet
(Streamlines, Gauge Pressure and Shear Stress)

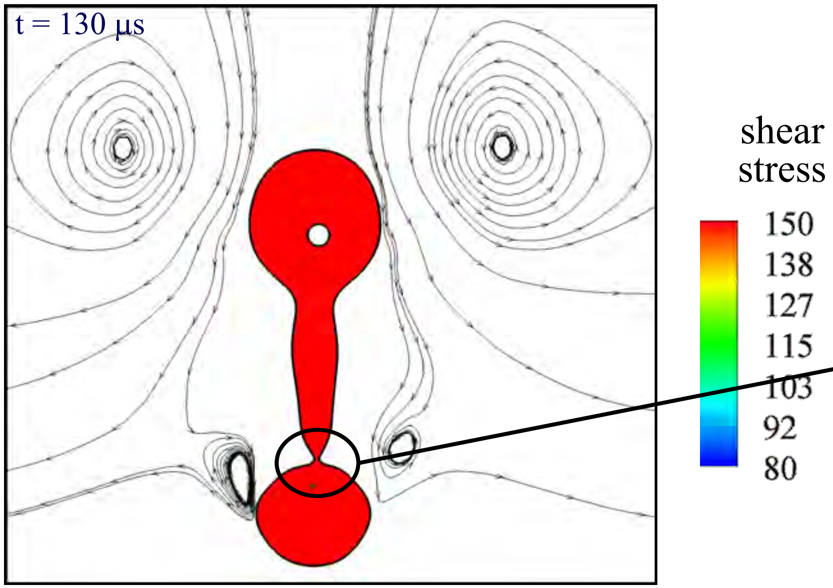
Diameter (μm)	Velocity (m/s)	p (atm)	We_g	Re_g
100	12	100	24	7609

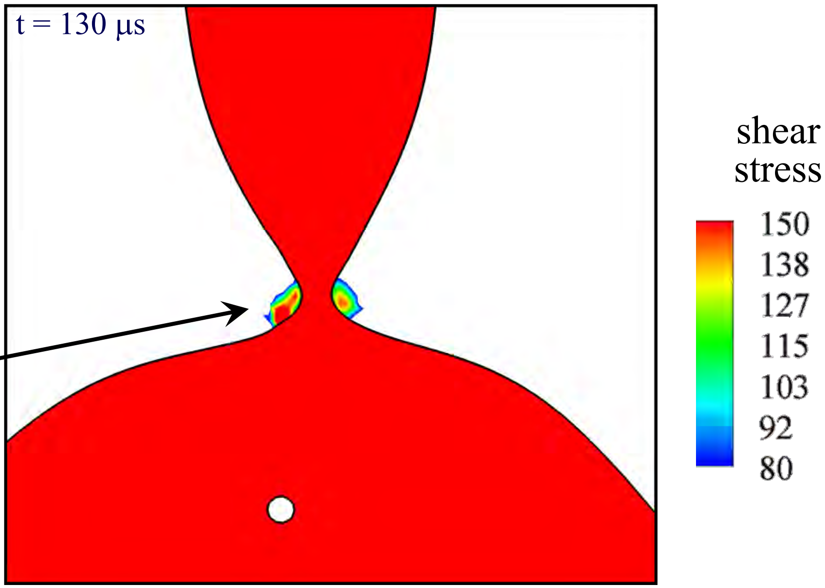


streamlines in moving coordinate system with droplet

Oscillatory Breakup of Water Droplet

(onset of breakup)

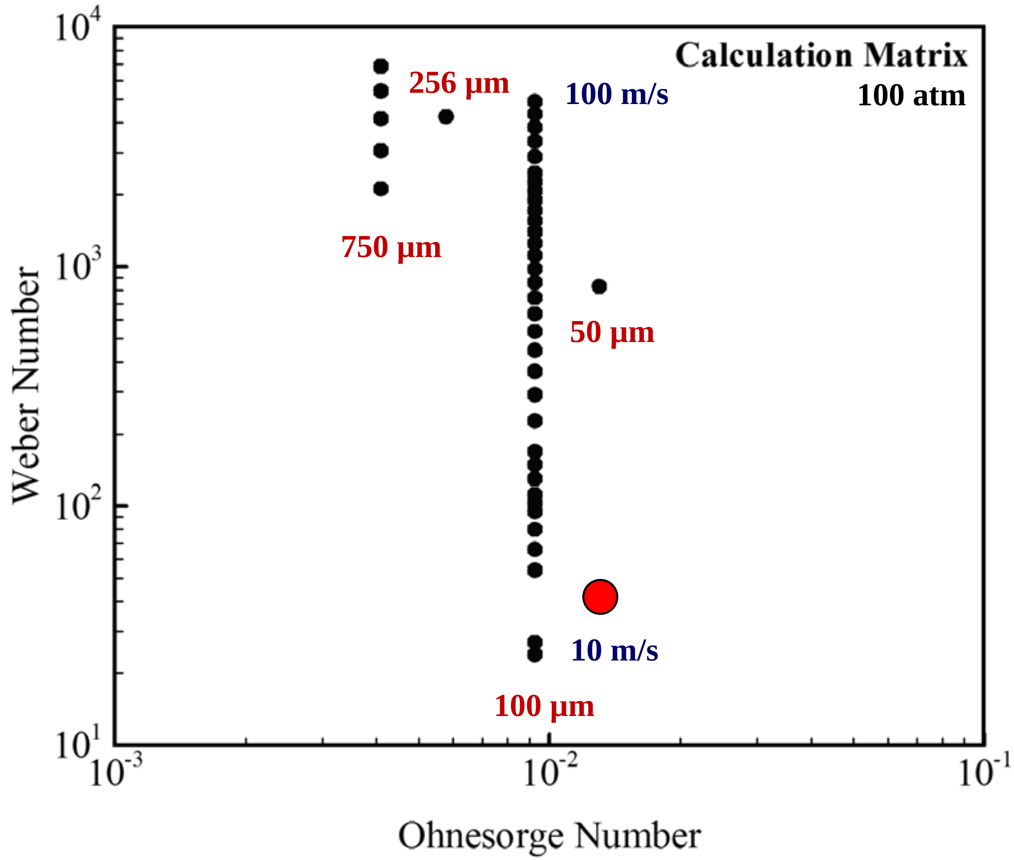




streamlines in fixed coordinate system

Bag Breakup

water droplet in air



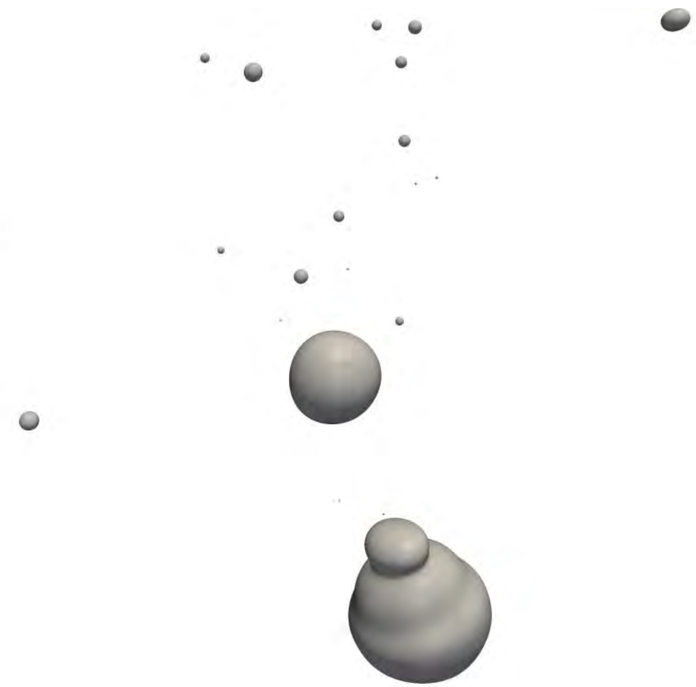
Bag Breakup
water droplet in air (100 atm)

Diameter (μm)	Velocity (m/s)	p (atm)	We_g	Re_g
50	20	100	33	6342

t = 1.0 μs

t = 10.0 μs

t = 57.8 μs



Lateral deformation and bag formation

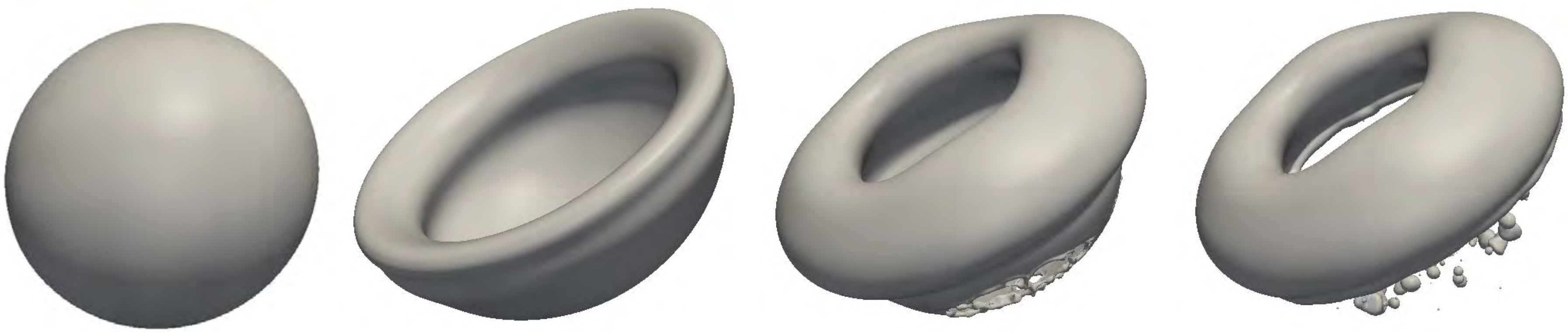
t = 19.7 μs

t = 21.0 μs

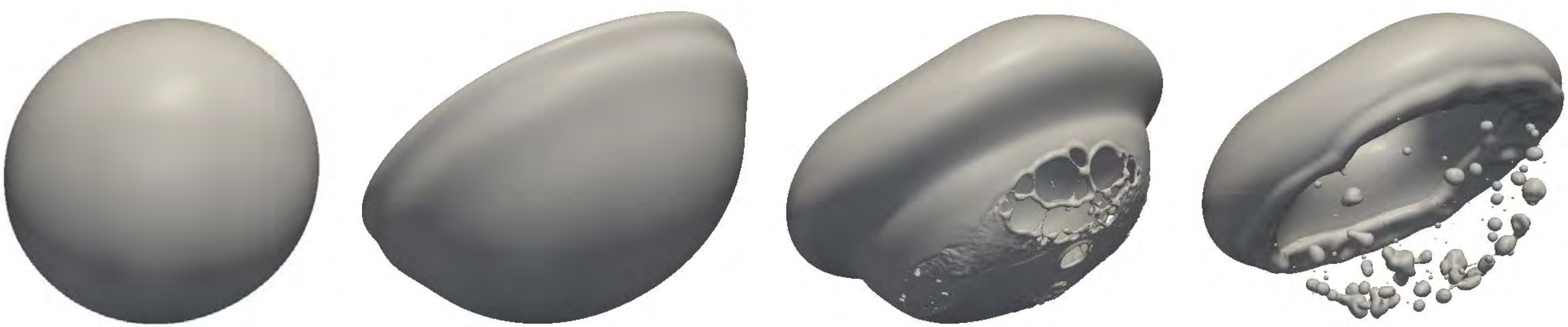
Bag breakup followed by rim breakup

Water - Air System – Bag Breakup (100 atm)

Diameter (μm)	Velocity (m/s)	We_g	Re_g
50	20	33	6342



Another view

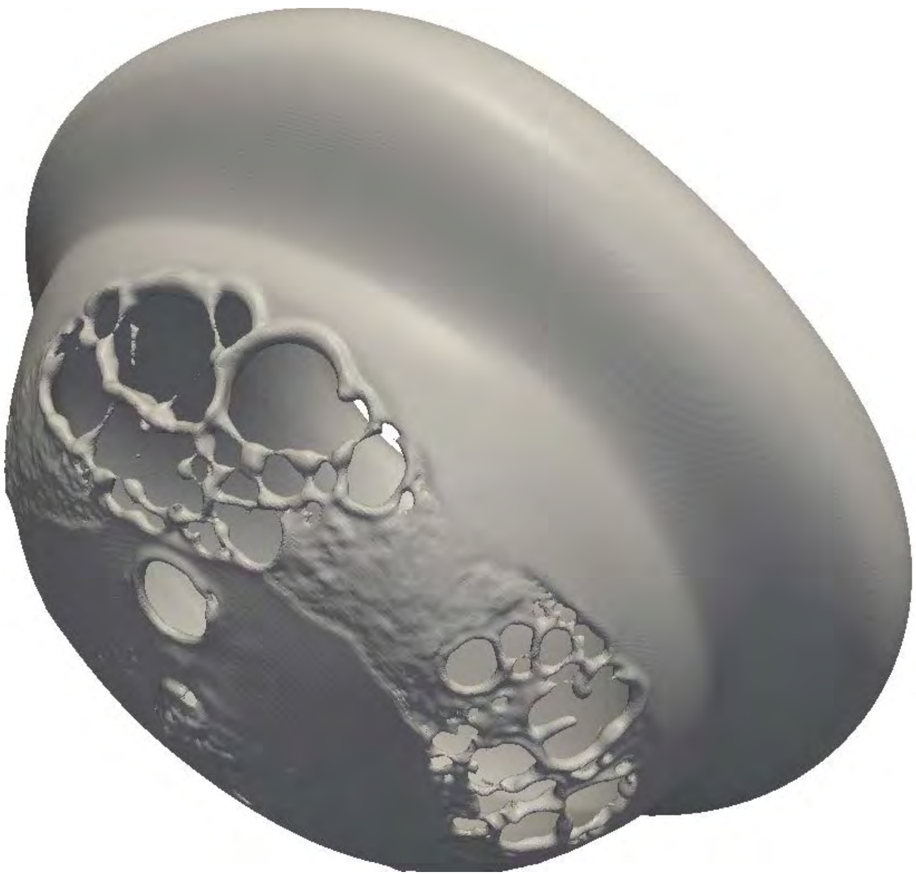


t = 1.00 μs t = 10.00 μs t = 20.00 μs t = 21.0 μs

Water - Air System – Bag Breakup (100 atm)

Diameter (μm)	Velocity (m/s)	We_g	Re_g
50	20	33	6342

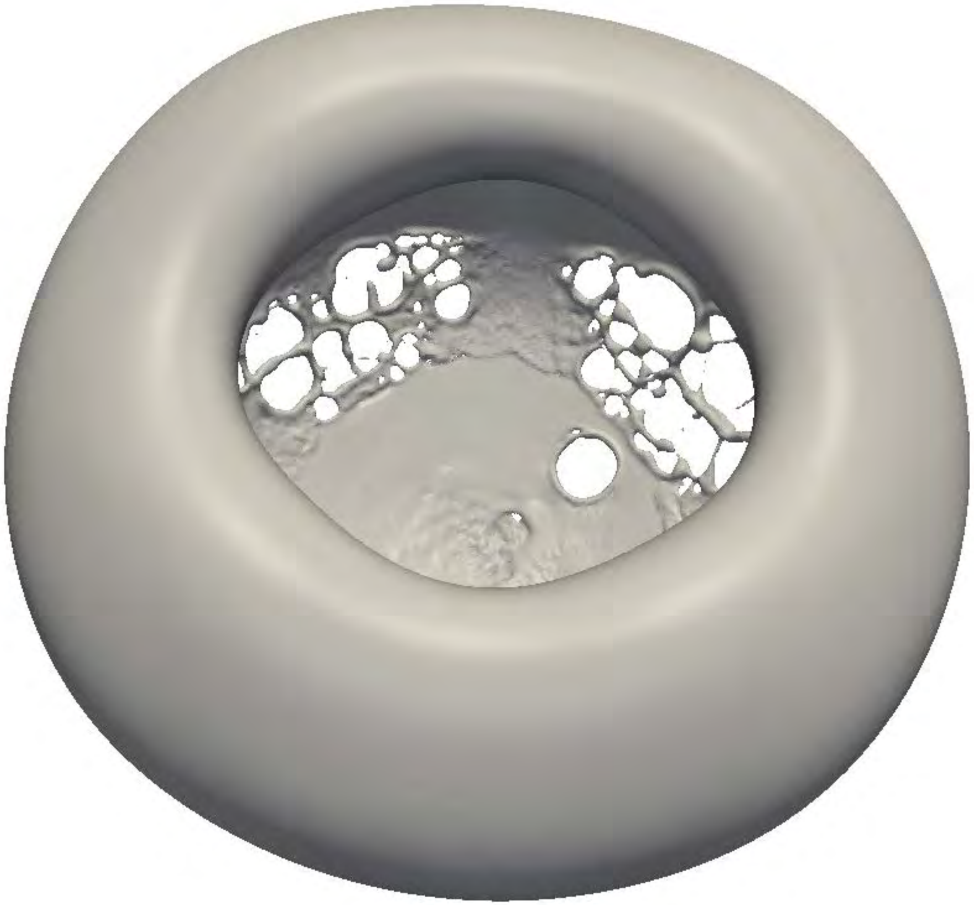
t = 20.00 μs



Water - Air System – Bag Breakup (100 atm)

Diameter (μm)	Velocity (m/s)	We_g	Re_g
50	20	33	6342

t = 20.00 μs



Water - Air System – Bag Breakup (100 atm)

Diameter (μm)	Velocity (m/s)	We_g	Re_g
50	20	33	6342

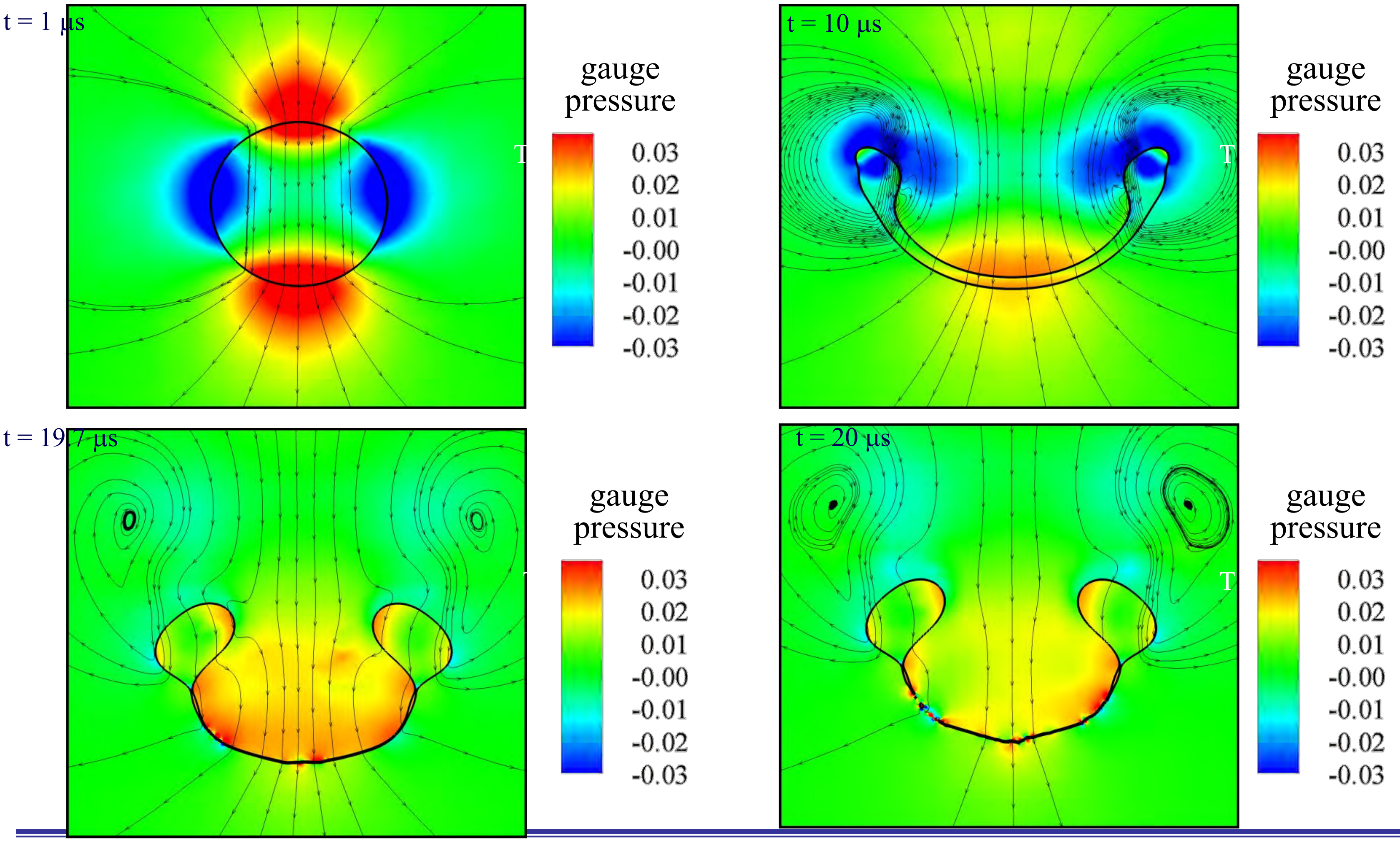
t = 20.00 μs

Bag Breakup of Water Droplet

(Streamlines and Gauge Pressure)

School of Aerospace Engineering

Diameter (μm)	Velocity (m/s)	p (atm)	We_g	Re_g
50	20	100	33	6342

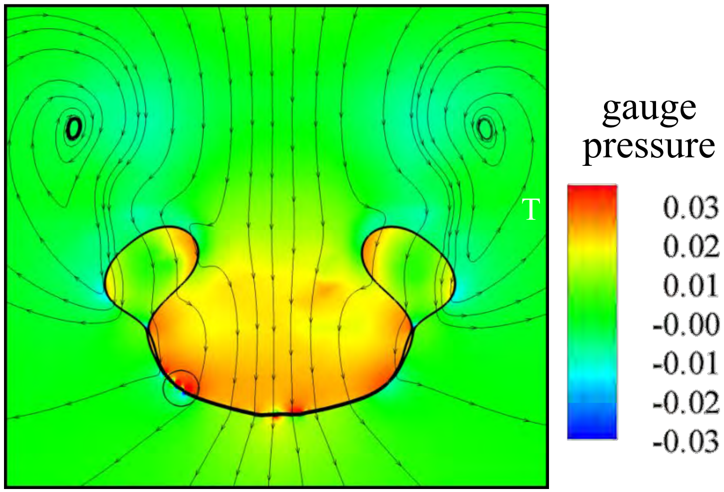


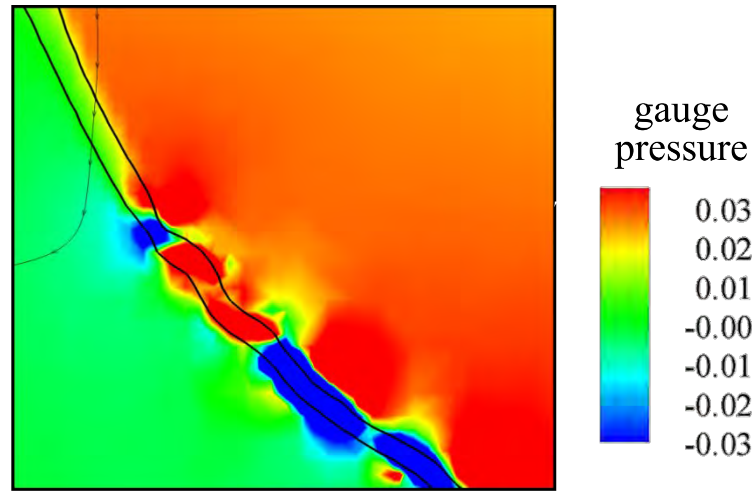
Gauge pressure = $(p - p_0)/(\text{density}*U^2)$

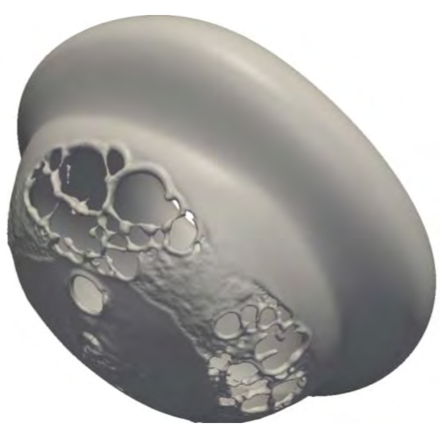
Khare & Yang/Georgia Tech

Onset of Breakup

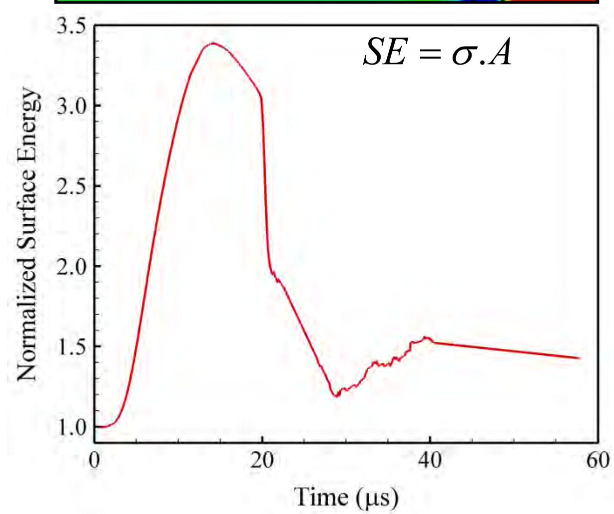
Diameter (μm)	Velocity (m/s)	p (atm)	We_g	Re_g
50	20	100	33	6342







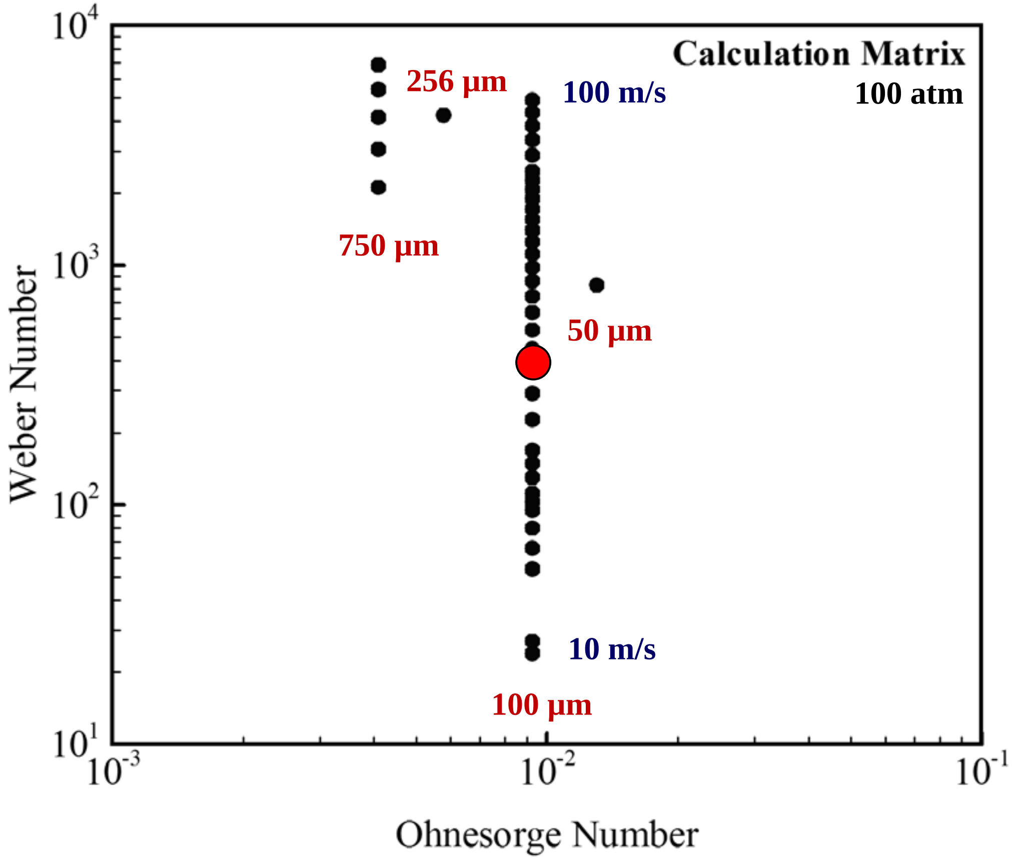
t = 19.7 μs



Gauge pressure = (p – p_0)/(density*U^2)

Multimode Breakup

water droplet in air



Multimode Breakup

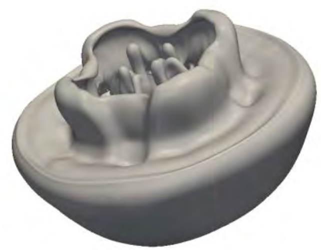
Water droplet in air (100 atm)

School of Aerospace Engineering

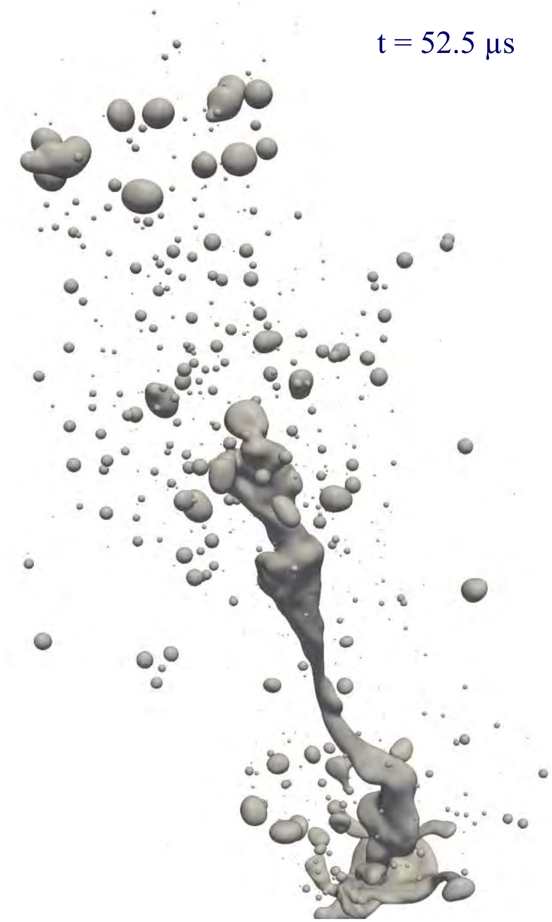
Diameter (μm)	Velocity (m/s)	p (atm)	We_g	Re_g
100	42	100	292	26635

t = 0.0 μs

t = 8.3 μs

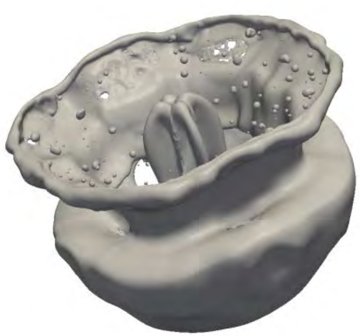


t = 52.5 μs

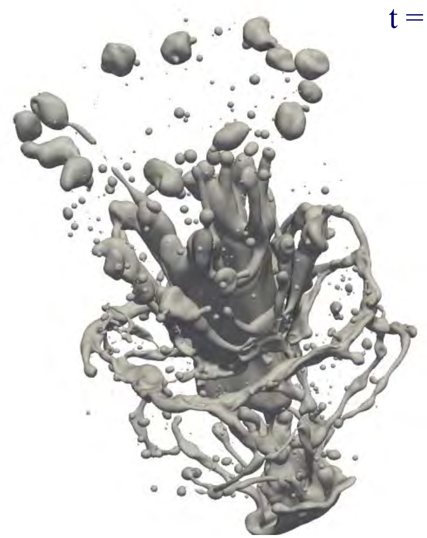


lateral deformation, bag, stem and lip formation

t = 11.9 μs



t = 19.0 μs



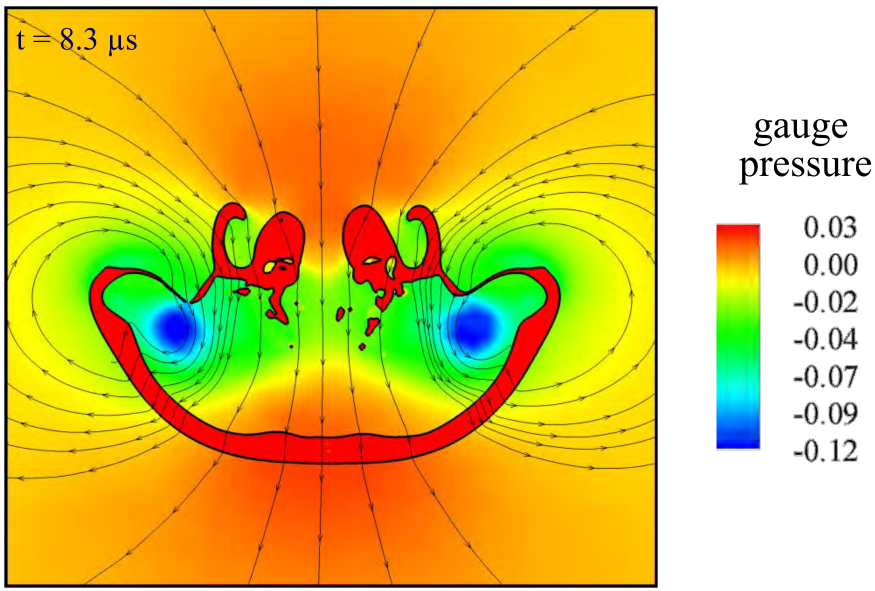
bag and lip thinning

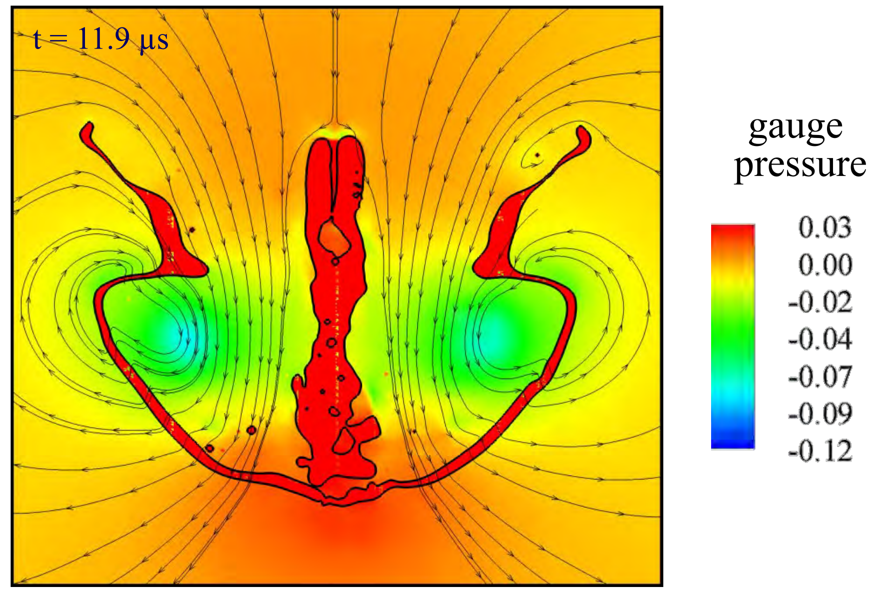
bag/lip breakup followed by rim and stem breakup

Multimode Breakup of Water Droplet
(Streamlines and Gauge Pressure around the onset of breakup)

School of Aerospace Engineering

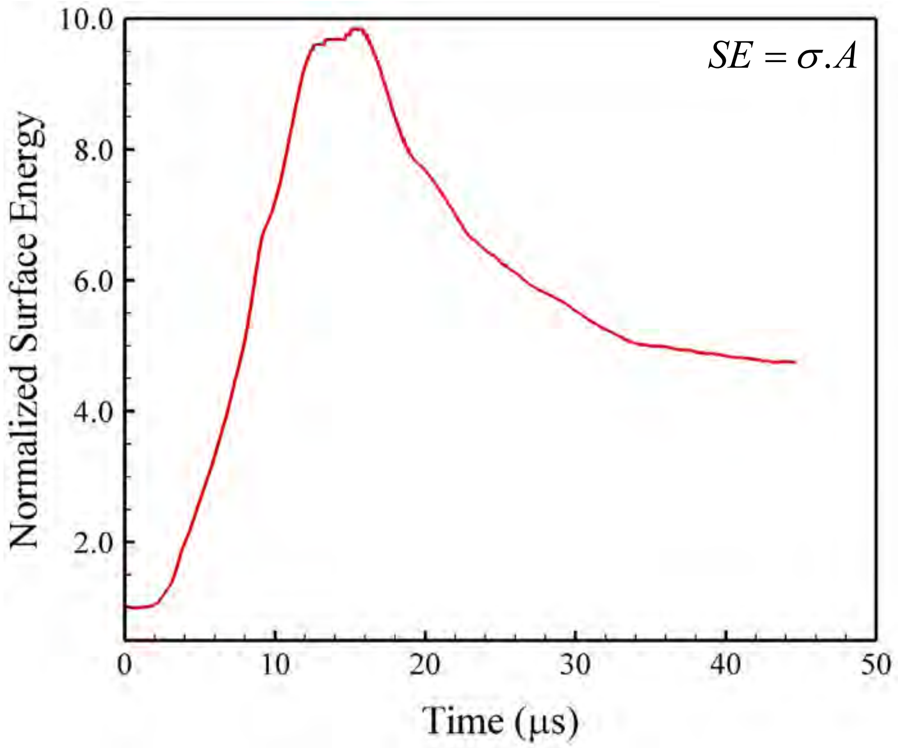
Diameter (μm)	Velocity (m/s)	p (atm)	We_g	Re_g
100	42	100	292	26635





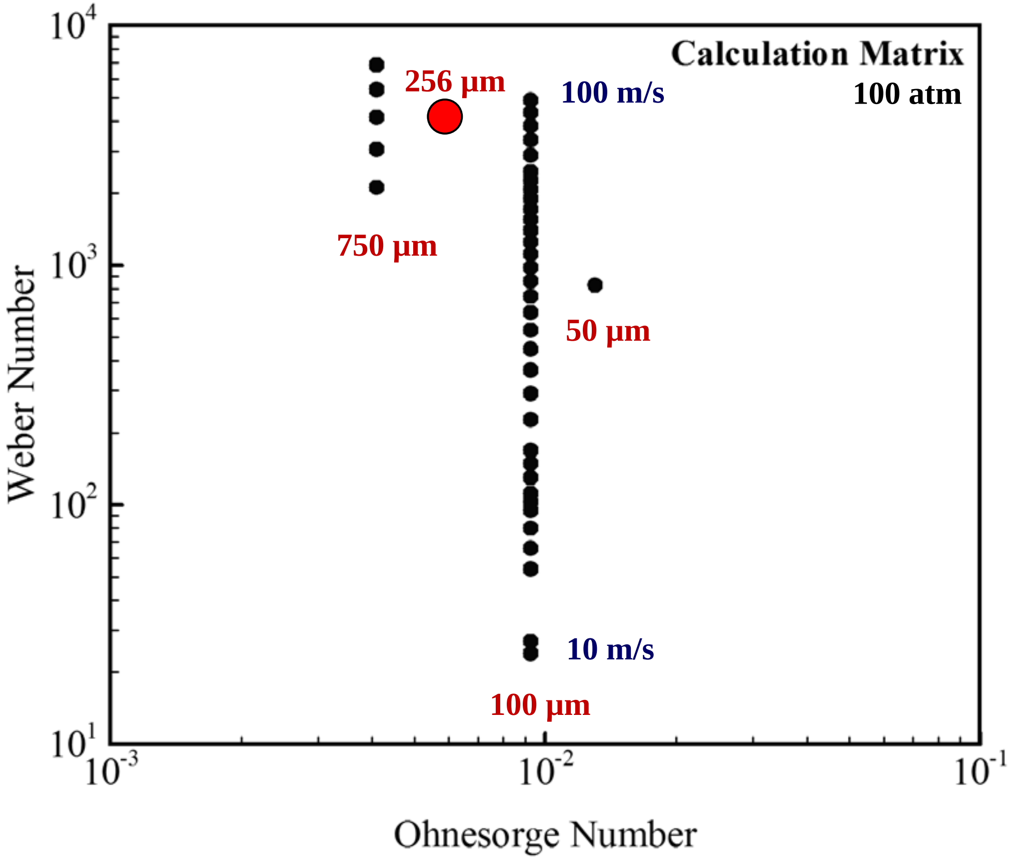
Gauge pressure = $(p - p_0)/(\text{density}^* U^2)$

Onset of Breakup : Energy Consideration



Shear Breakup

water droplet in air



Shear Breakup
Water droplet in air (100 atm)

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Diameter (μm)	Velocity (m/s)	p (atm)	We_g	Re_g
256	100	100	4237	162350

t = 0.30 μs

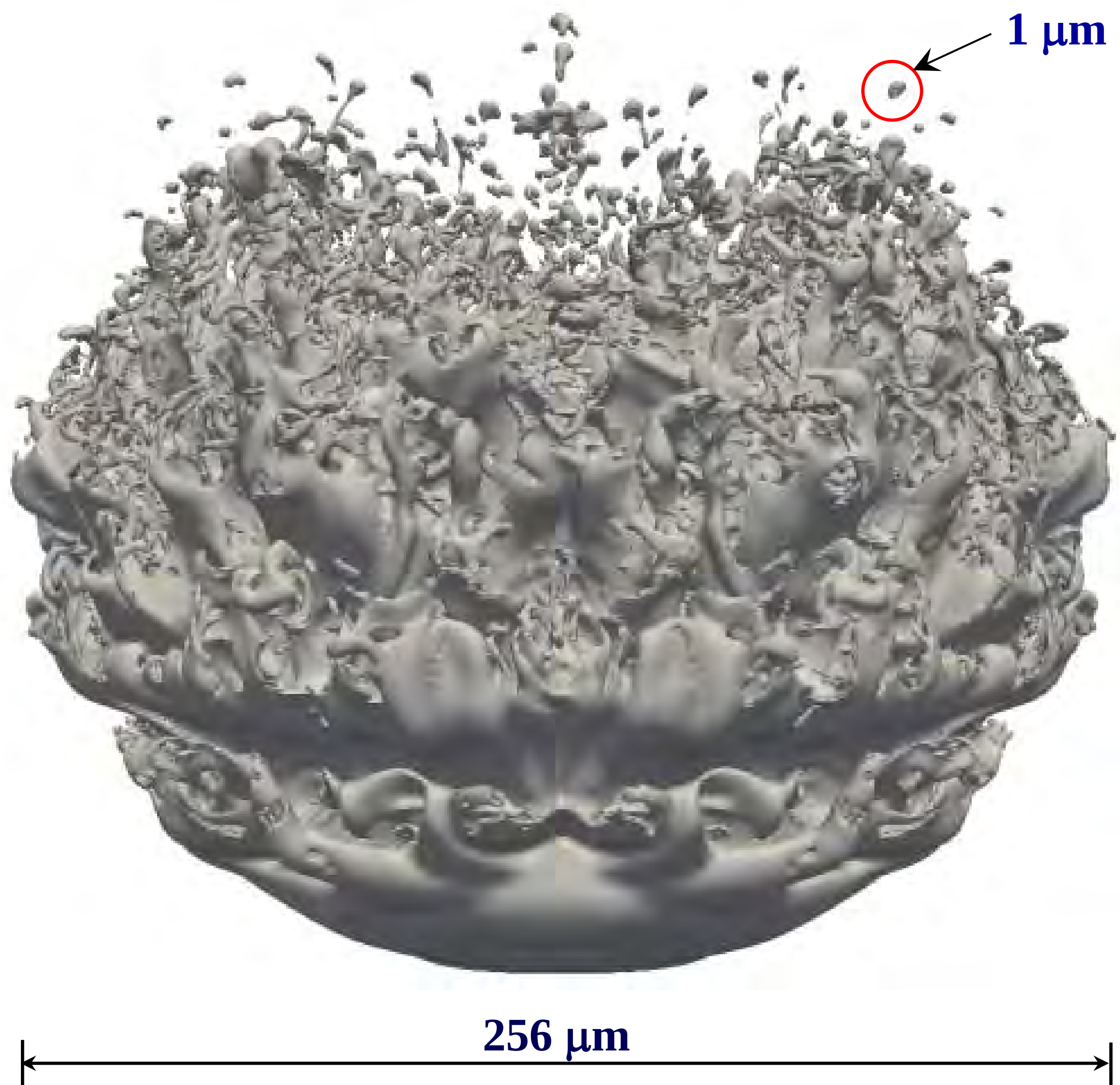
t = 0.92 μs

t = 1.84 μs

t = 2.46 μs

Shear Breakup - Length Scales
Water droplet in air (100 atm)

School of Aerospace Engineering

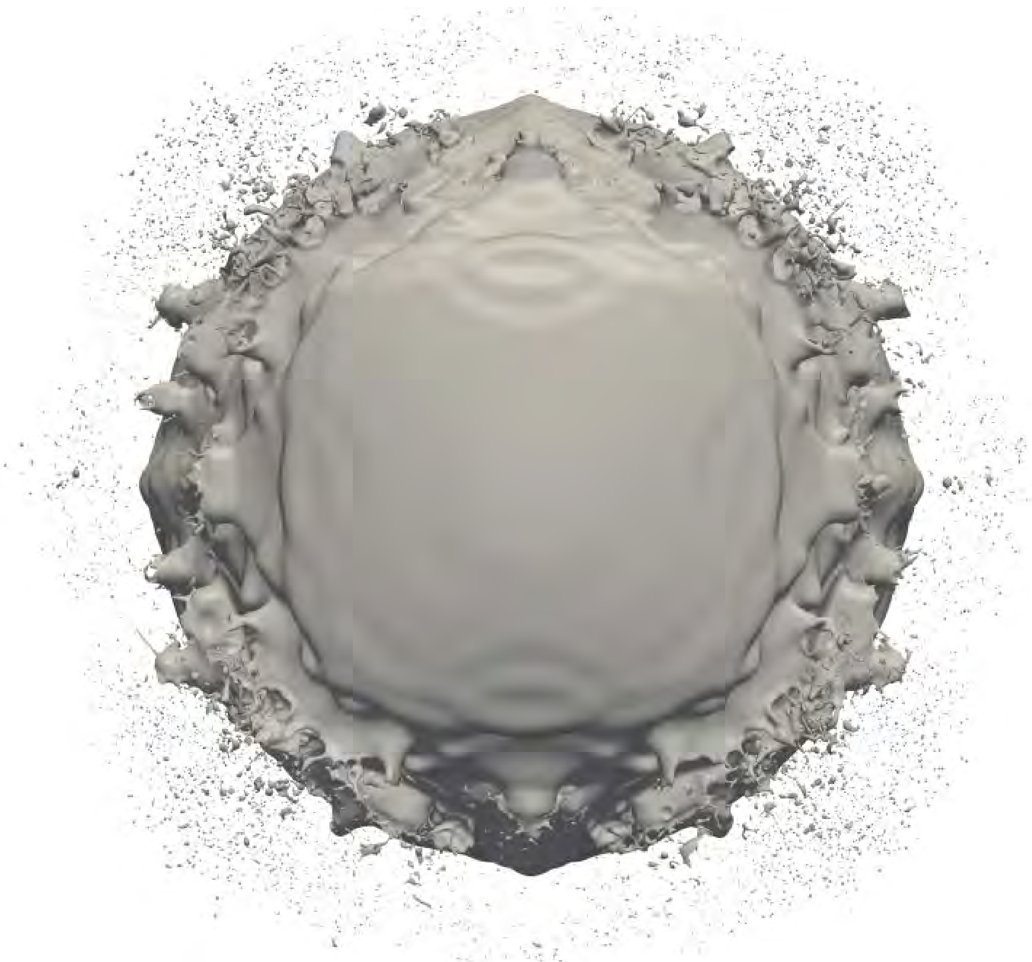


Shear Breakup - Present Simulation

water droplet in air (1 atm)

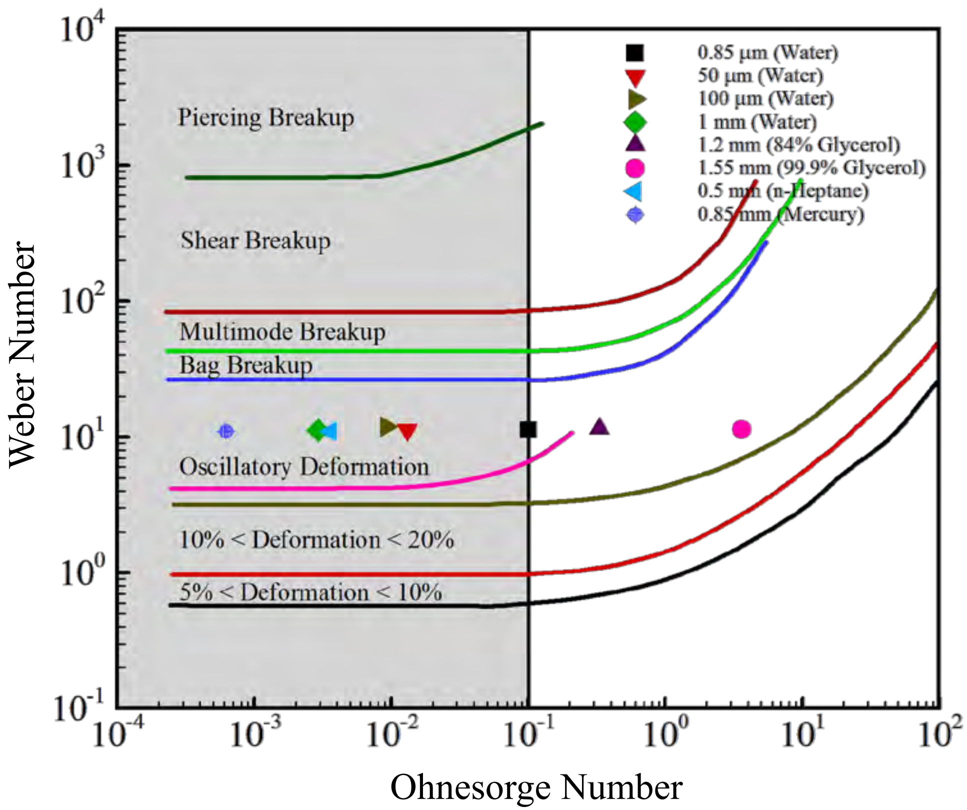
Features:

- Sheet thinning mechanism
- Rayleigh-Taylor waves due to acceleration of a higher density fluid in a lower density gas.



We = 112, *Oh* = 0.0034

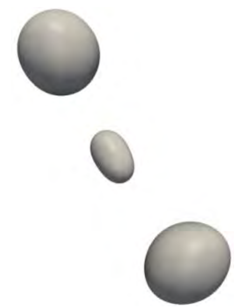
Breakup Regime Diagram (1 atm)



$$Oh = \frac{\mu_l}{\sqrt{\rho_l D \sigma}}$$

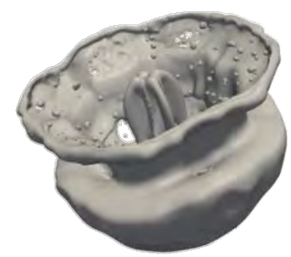
$$We = \frac{\rho_g U^2 D}{\sigma}$$

Oscillatory breakup



Bag breakup

Multimode breakup

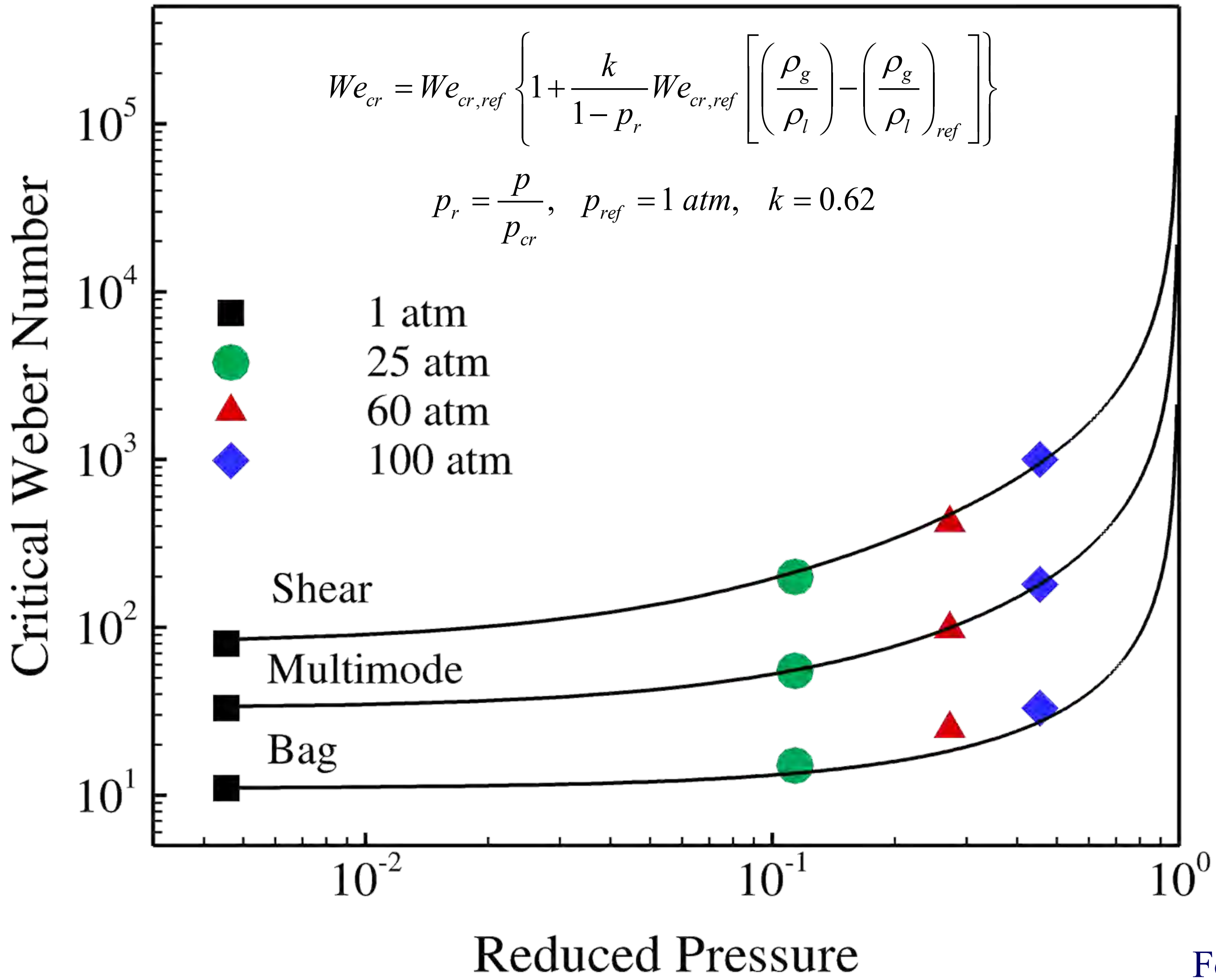


Shear breakup

Fluid (in air)	ρ (kg/m³)	μx10⁴ (kg/m-s)	σx10³ (N/m)
Water	1000	7.89	72.8
n-Heptane	683	3.94	20.0
Mercury	13600	15.0	475.0
Glycerol (84%)	1219	1000	63.2
Glycerol (99.9%)	1260	12500	62.0

L.-P. Hsiang & G. M. Faeth, Drop deformation and breakup due to shock wave and steady disturbances, IJMF, 1995.

Generalized Regime Diagram



For *Oh* < *0.1*

Breakup Modes

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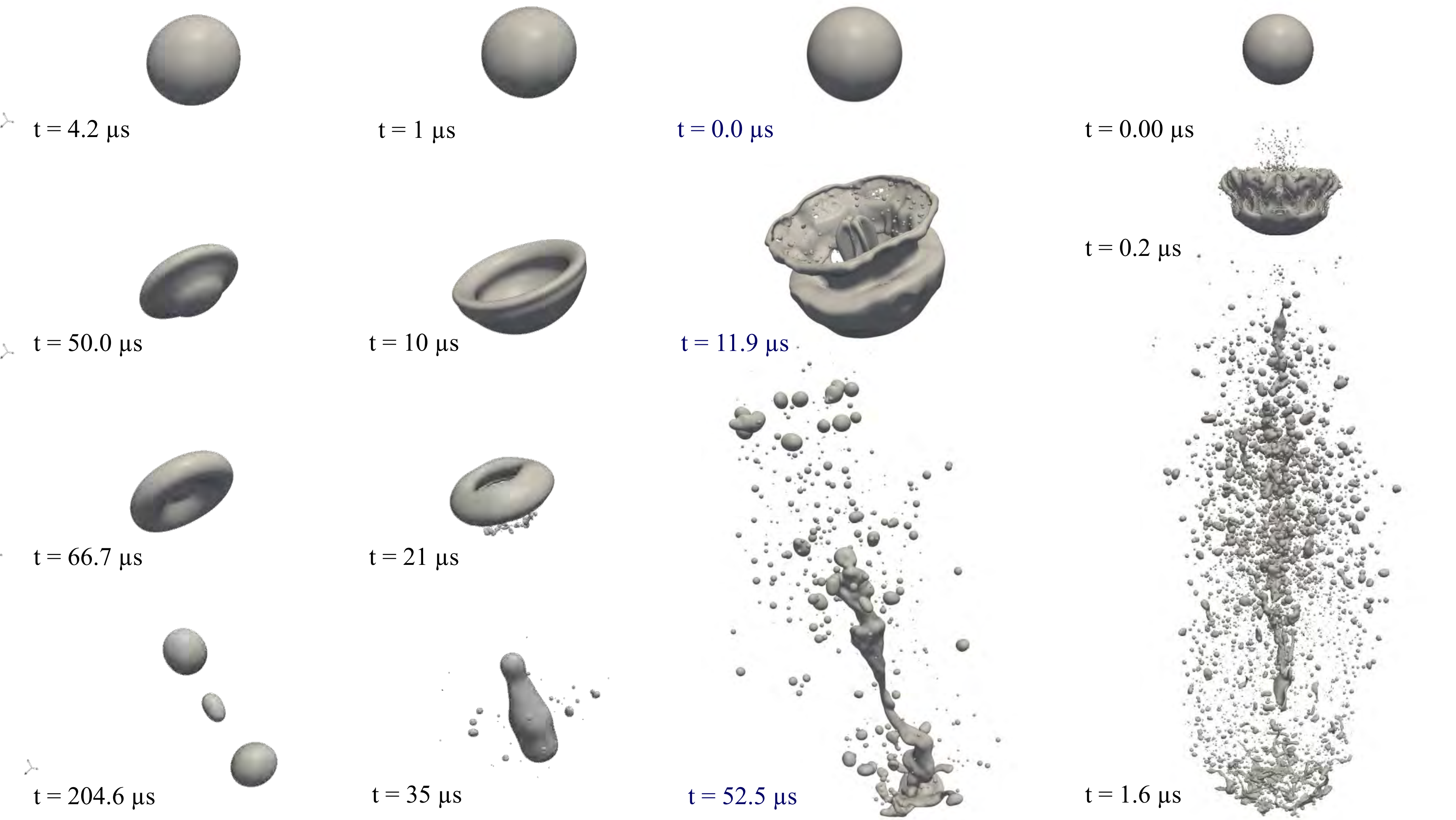
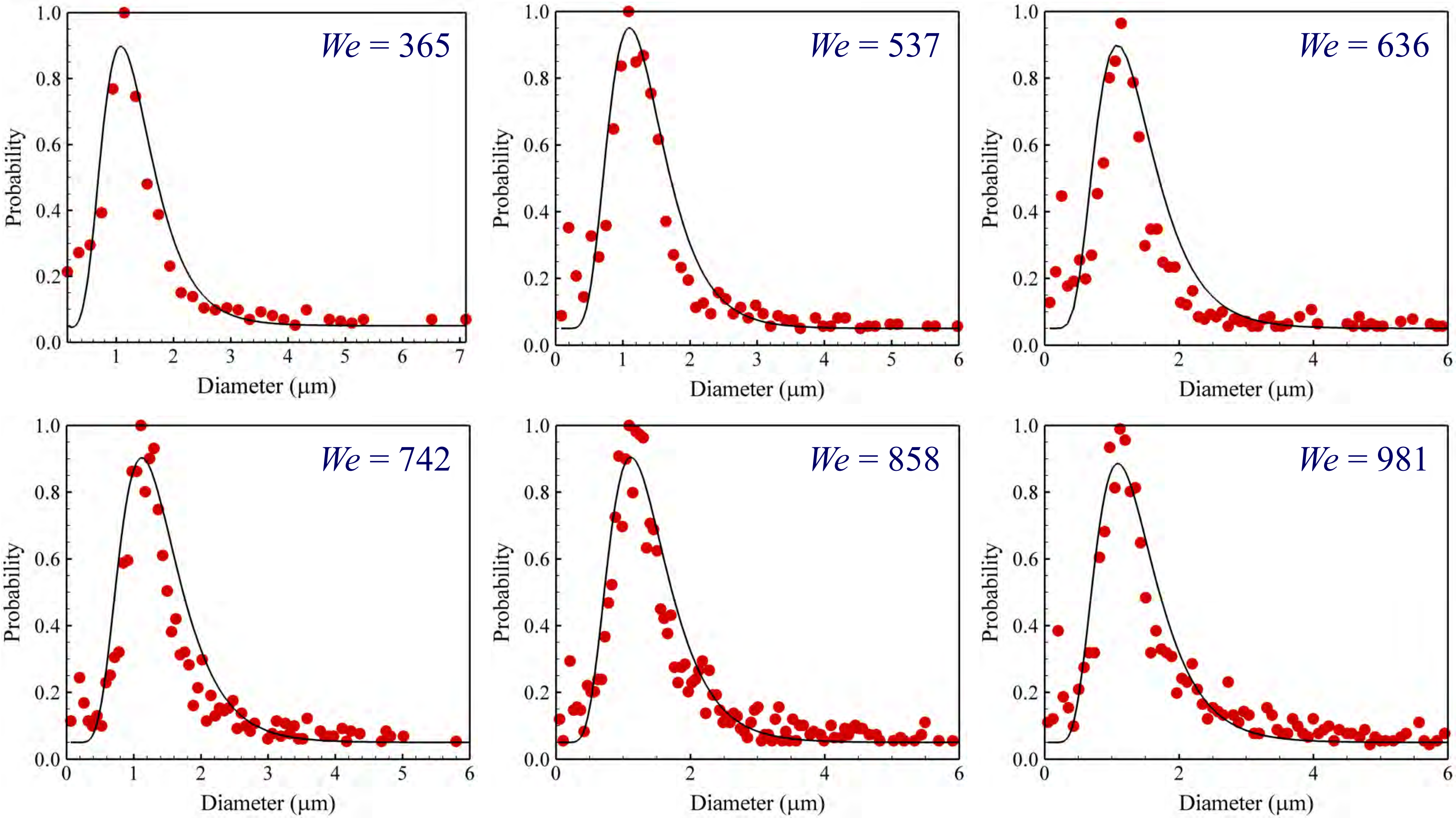
Oscillatory Breakup | **Bag Breakup** | **Multimode Breakup** | **Shear Breakup**



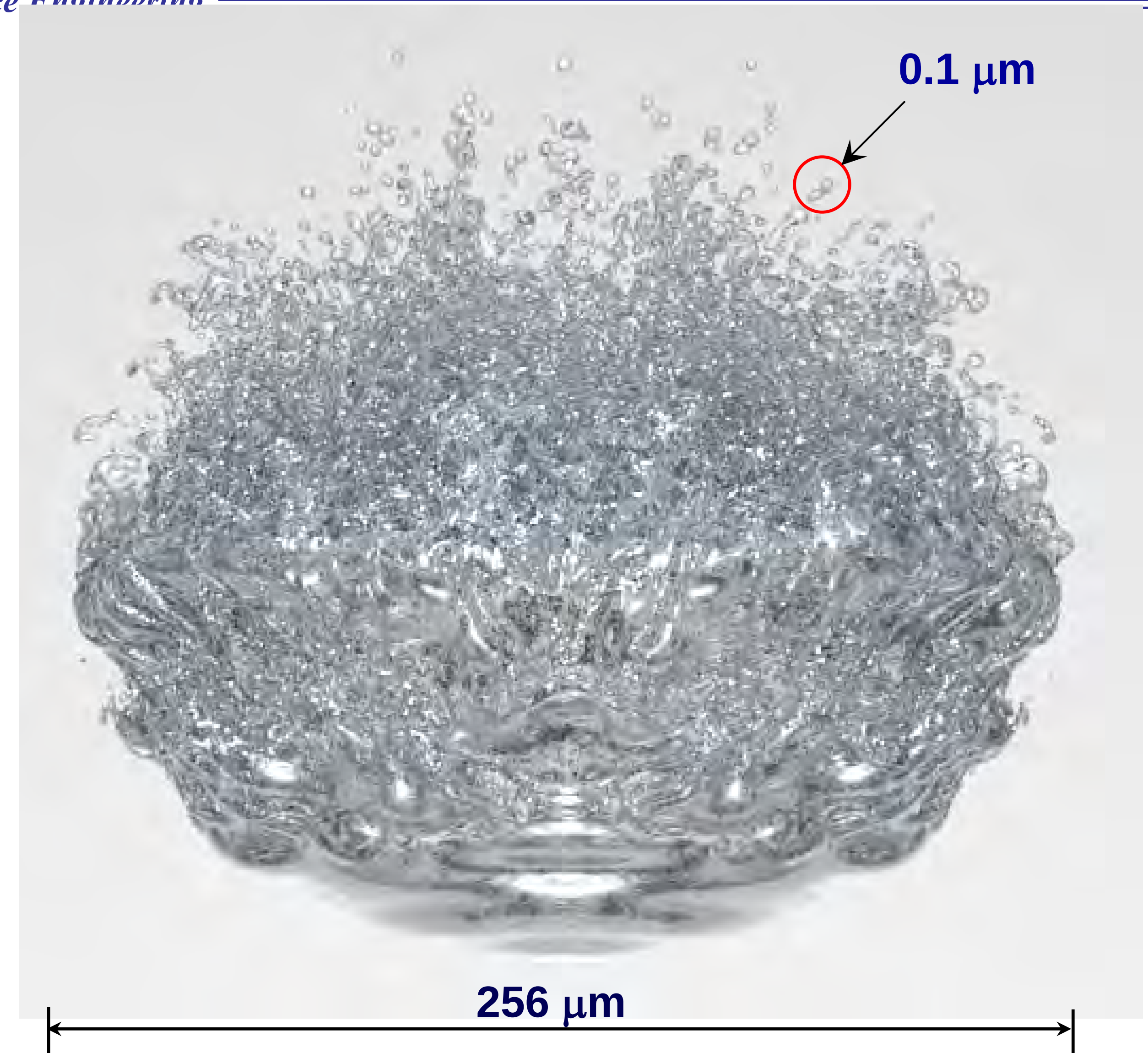
We = 24 | **We = 33** | **We = 292** | **We = 1400**

Child Droplet Distribution



PDF of child droplet size distribution for *We* > 300

Shear Breakup - Length Scales
water droplet in air (100 atm)



文翰

寿比南山

一百岁生日时，請我们大家都来！

Tony:

All the best of luck!

We all will come back to celebrate your 100th birthday!