Morphology of droplets in turbulent flows

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Ianto Cannon, Giovanni Soligo, and Marco E. Rosti
Okinawa Institute of Science and Technology

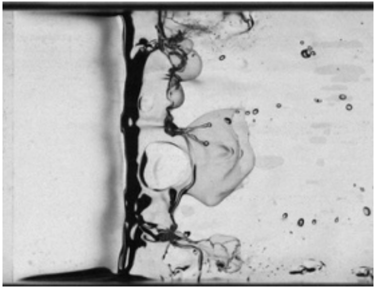
We care about droplet morphology

CO_2 absorption[a]

Wave breaking on the coast of Okinawa[b].

[a]Merlivat, L., & Memery, L. (1983). *J. Geophys. Res.-Oceans, 88*(C1), 707–724.
[b]Photo credit: Linda Gietka

Droplet breakup during cough[a]



1mm water & glycerol film with 15m/s airflow.

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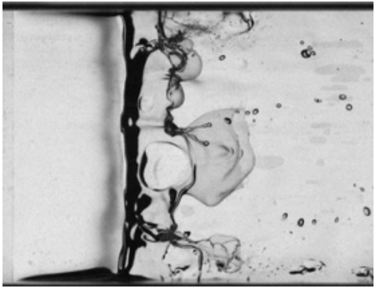

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What is the morphology of droplets in turbulence?

How do surfactants affect morphology?

Numerical method

We use the in-house solver *Fujin*.
Fluid motion,

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \right] + \nabla \cdot (\tau_c f_\sigma) + \mathbf{f_s},$$
$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

Droplet motion[a],

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = 0, \tag{2}$$

Surfactant motion[b],

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \nabla \cdot (M_\psi \nabla \mu_\psi), \tag{3}$$

Surface tension[c],

$$f_\sigma = \max[\sigma_{min}, \sigma_0(1 + \beta_s \log(1 - \psi))]. \tag{4}$$

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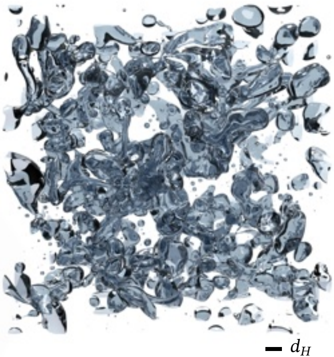
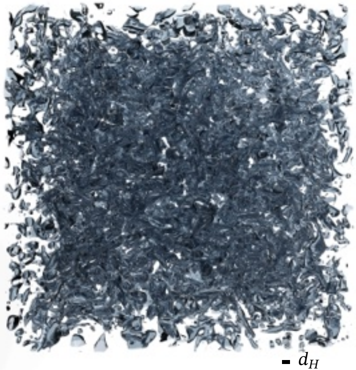
[a] Ii, S., Sugiyama, K., Takeuchi, S., Takagi, S., Matsumoto, Y., & Xiao, F. (2012). *Journal of Computational Physics, 231*(5), 2328–2358.
[b] Engblom, S., Do-Quang, M., Amberg, G., & Tornberg, A. (2013). *Commun. Comput. Phys., 14*(4), 879–915.
[c] Muradoglu, M., & Tryggvason, G. (2008). *Journal of Computational Physics, 227*(4), 2238–2262.

Simulation setup

- Tri-periodic domain with $500 \times 500 \times 500$ grid points.
- Six simulations with three values of surface tension, and two surfactant concentrations.
- Hinze-scale[d] $d_H \equiv 0.725\sigma^{3/5}\rho^{-3/5}\epsilon^{-2/5}$.

case		$\langle\phi\rangle$	$\langle\psi\rangle$	We_e	d_H/L
C10	●	0.1	0	**9.91**	**0.0560**
C20	●	0.1	0	20.0	0.0373
C40	●	0.1	0	39.3	0.0252
S05	◆	0.1	0.1	12.7	0.0489
S10	◆	0.1	0.1	25.8	0.0338
S20	◆	0.1	0.1	**49.5**	**0.0232**





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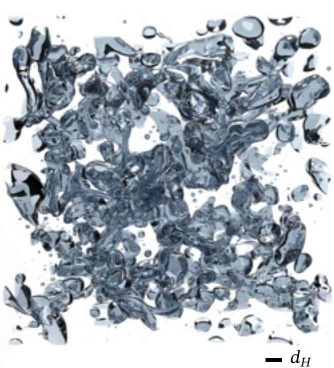

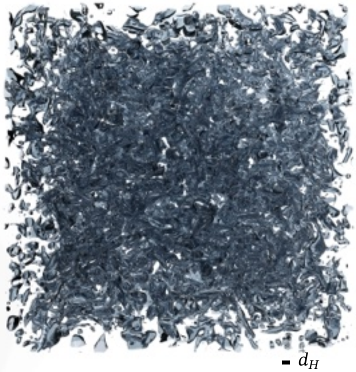

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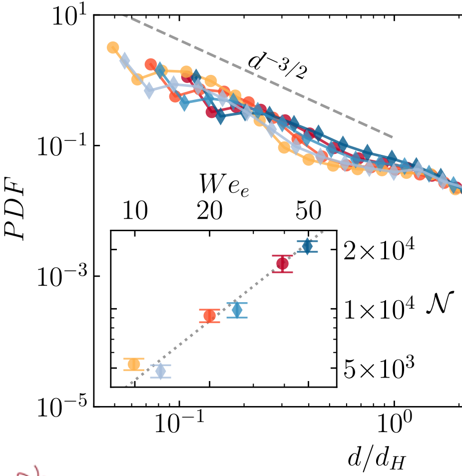
Counting droplets.



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- We use a flood-fill algorithm to count the droplets[a].
- Surface tension $\sigma\downarrow$, number of droplets $\mathcal{N}\uparrow$.
- Define a volume-based diameter for each droplet, $d \equiv (6V/\pi)^{1/3}$.
- $d < d_H$: coalescence.
- $d > d_H$: breakup[b].

[a] Newman, W. M., & Sproull, R. F. (Eds.). (1979). McGraw-Hill, Inc.

[b] Deane, G. B., & Stokes, M. D. (2002). *Nature, 418*(6900), 839–844.

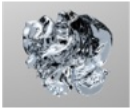
What shape are the droplets?

←1.0→

↑ 0.9 ↓

←1.0→

↑ 0.5 ↓



Aspect ratio $\sqrt{I_1/I_3}$	0.946	0.633	0.905
Sphericity d/d_A	0.999	0.965	0.701

- I_1 and I_3 are the smallest and largest moments of inertia.
- Area-based diameter for each droplet, $d \equiv \sqrt{A/\pi}$.

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			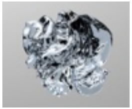
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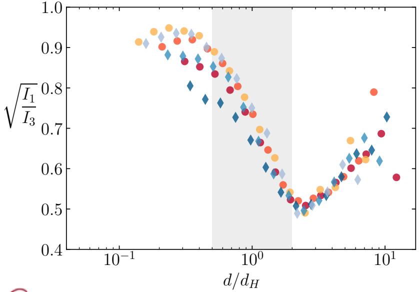

- I_1 and I_3 are the smallest and largest moments of inertia.
- Area-based diameter for each droplet, $d \equiv \sqrt{A/\pi}$.
- $d << d_H$ aspect ratio → 1.
- $d \approx d_H$ droplets are extended.
- $d >> d_H$ aspect ratio → 1.

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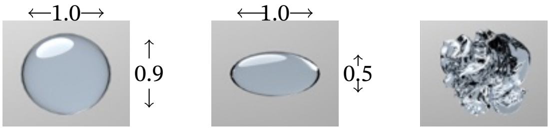

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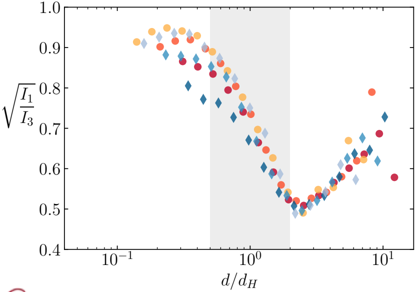

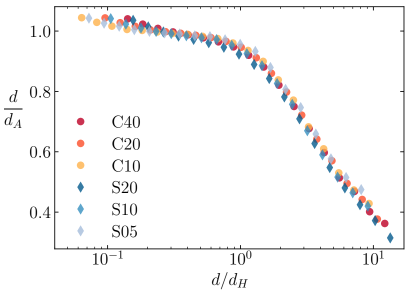

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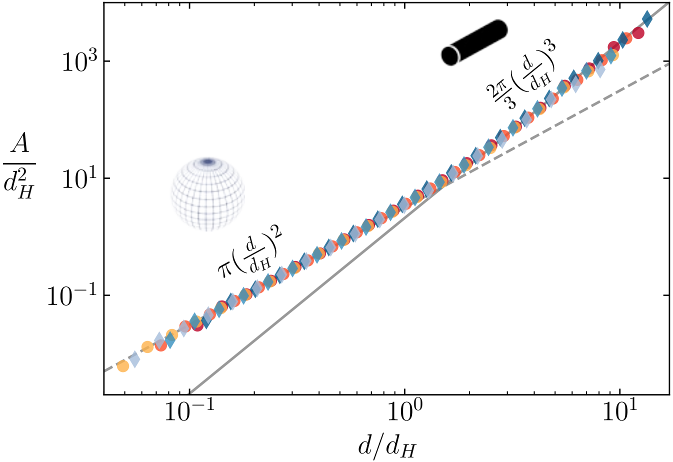
- $d > d_H$ area ↑.

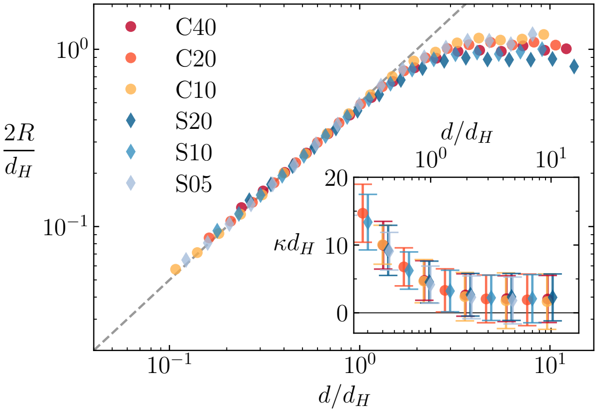
What is the area of the droplets?

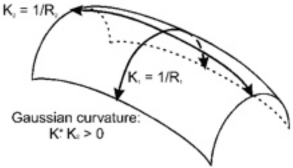


- $d < d_H$: spheroids.
- $d > d_H$: filaments with diameter d_H.

Interface curvature

Curvature $\kappa = \kappa_1 + \kappa_2 = 1/R$.

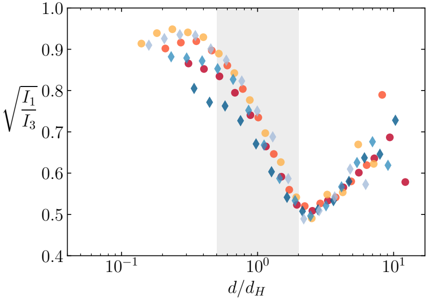




- $d < d_H$: $R = d/4$.
- $d > d_H$: $R = d_H/2$, with regions of negative curvature.

Recap

- The large droplets are filamentous.



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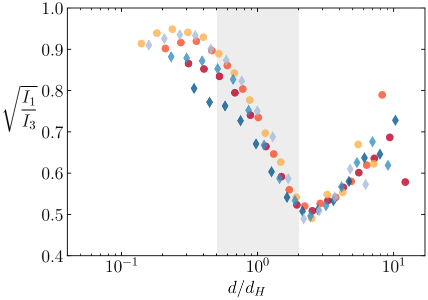

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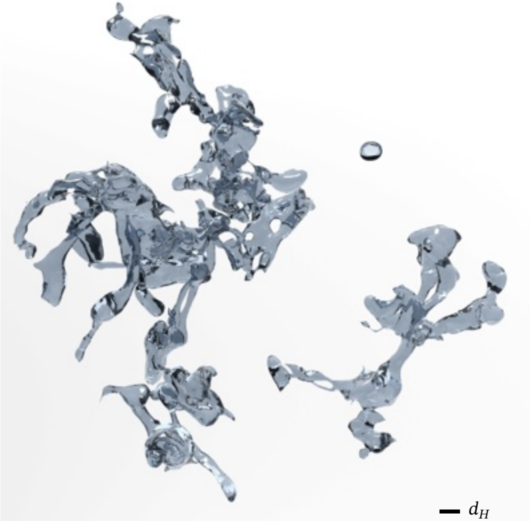
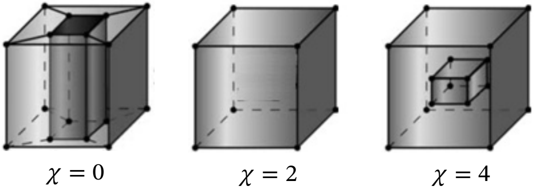


How to count the number of handles?

We compute the Euler characteristic[e] of the droplet interfaces.

$$\chi = n - e + f \quad (5)$$

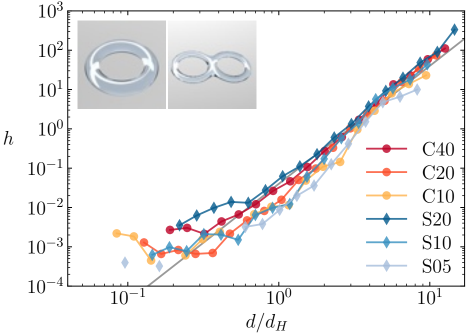


This gives the number of handles[f] h and voids v.

$$\chi = 2 + 2v - 2h. \quad (6)$$

[e] Massey, W. S. (1997). Springer.
[f] Mendoza, R., Thornton, K., Savin, I., & Voorhees, P. (2006). *Acta Mater., 54*(3), 743–750.

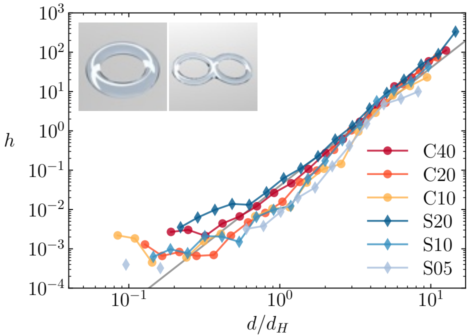
How many handles and voids are there?



$$h = 0.04(d/d_H)^3$$

- Constant number of handles per unit length of filament.

How many handles and voids are there?



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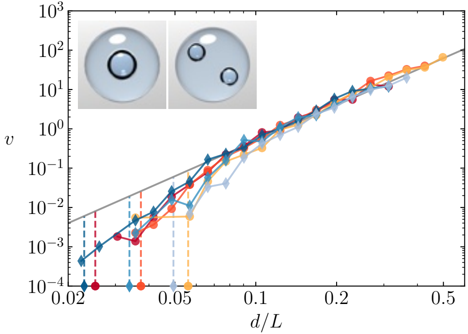
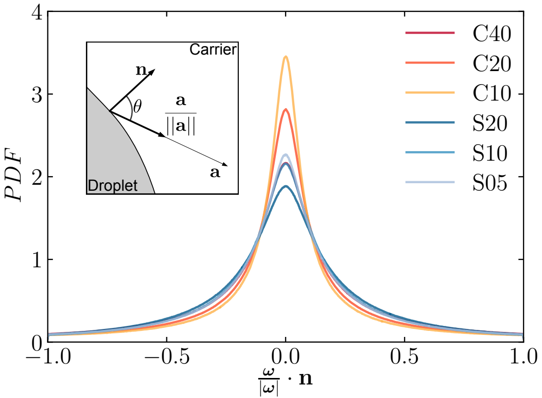


$$v = 500(d/L)^3$$

- Constant number of voids per unit volume of droplet.

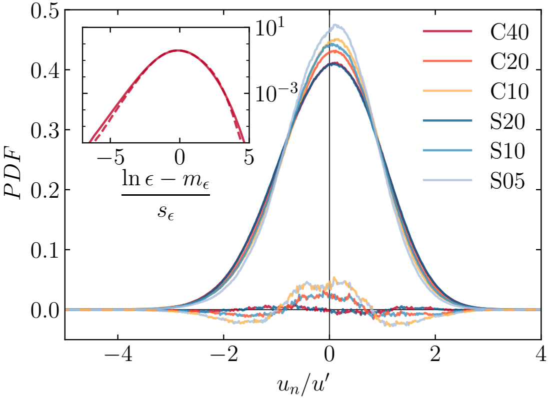
Vorticity at the interface



- Vorticity $\boldsymbol{\omega} = \nabla \times \boldsymbol{u}$.
- Normal to the interface $\boldsymbol{n}$.
- Vorticity is mostly tangential to the interface[a].
- Surface tension ↓, effect ↓.
- Surfactants increase velocity gradients tangential direction.

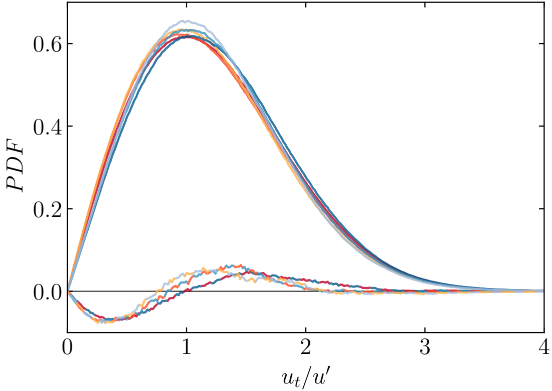
[a] Shao, C., Luo, K., Yang, Y., & Fan, J. (2018). *International Journal of Multiphase Flow, 107*, 263–274.

Flow normal to interface



- Extreme inward velocities are more likely than outward.
- m_ε and s_ε are the mean and standard deviation of the dissipation ε.
- Surfactant suppresses large normal velocities.

Flow tangential to interface



- Surfactant induces large tangential velocities.

Conclusions

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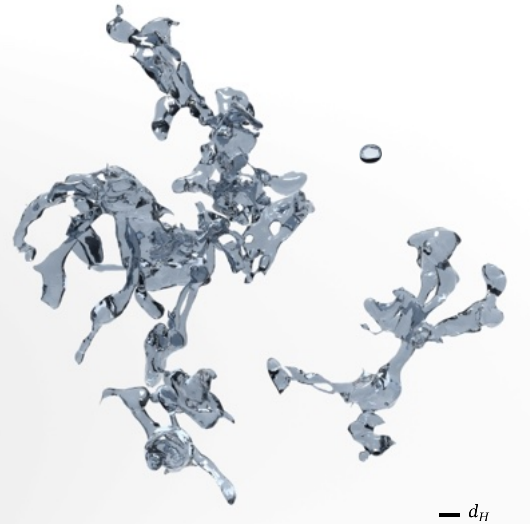

[a] Cannon, I., Soligo, G., & Rosti, M. E. (2023). *arXiv:2307.15448*.

Bibliography I

- Cannon, I., Soligo, G., & Rosti, M. E. (2023). Morphology of clean and surfactant-laden droplets in homogeneous isotropic turbulence. *arXiv:2307.15448.*
- Deane, G. B., & Stokes, M. D. (2002). Scale dependence of bubble creation mechanisms in breaking waves. *Nature, 418*(6900), 839–844.
- Engblom, S., Do-Quang, M., Amberg, G., & Tornberg, A. (2013). On diffuse interface modeling and simulation of surfactants in two-phase fluid flow. *Commun. Comput. Phys., 14*(4), 879–915.
- Hinze, J. O. (1955). Fundamentals of the hydrodynamic mechanism of splitting in dispersion processes. *AIChE Journal, 1*(3), 289–295.
- Ii, S., Sugiyama, K., Takeuchi, S., Takagi, S., Matsumoto, Y., & Xiao, F. (2012). An interface capturing method with a continuous function: The THINC method with multi-dimensional reconstruction. *Journal of Computational Physics, 231*(5), 2328–2358.
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- Massey, W. S. (1997). *A basic course in algebraic topology* (Corr. 3rd print). Springer.
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Bibliography II

Merlivat, L., & Memery, L. (1983). Gas exchange across an air-water interface: Experimental results and modeling of bubble contribution to transfer. *J. Geophys. Res.-Oceans, 88*(C1), 707–724.

Muradoglu, M., & Tryggvason, G. (2008). A front-tracking method for computation of interfacial flows with soluble surfactants. *Journal of Computational Physics, 227*(4), 2238–2262.

Newman, W. M., & Sproull, R. F. (Eds.). (1979). *Principles of interactive computer graphics (2nd ed.)*. McGraw-Hill, Inc.

Shao, C., Luo, K., Yang, Y., & Fan, J. (2018). Direct numerical simulation of droplet breakup in homogeneous isotropic turbulence: The effect of the Weber number. *International Journal of Multiphase Flow, 107*, 263–274.