Phase-field simulation of Rayleigh instability on a fibre

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A B S T R A C T

In this paper, we present a phase-field method for Rayleigh instability on a fibre. Unlike a liquid column, the evolutionary dynamics of a liquid layer on a fibre depends on the boundary condition at the solid–liquid interface. We use a Navier–Stokes–Cahn–Hilliard system to model axisymmetric immiscible and incompressible two-phase flow with surface tension on a fibre. We solve the Navier–Stokes equation using a projection method and the Cahn–Hilliard equation using a nonlinearly stable splitting method. We present computational experiments with various thicknesses of liquid thread and fibre. The numerical results indicate that the size of the satellite droplet decreases as the thicknesses of the thread and fibre increase.

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1. Introduction

The coating problem of a cylindrical fibre with a liquid film has been intensively studied because of its relation with technological and industrial processes, i.e., the coating of conducting cables with isolating films (González et al., 2010). However, compared to a lot of literature on the simulations of the break-up of a liquid thread under the Rayleigh instability (RI) (Chakrabarti et al., 2017; Gopan and Sarith, 2014; Joshi et al., 2016; Vega et al., 2010; Yan et al., 2015) and references therein, there are only few numerical works on the RI on a fibre (González et al., 2010; Haefner et al., 2015; Mead-Hunter et al., 2012). Fig. 1 shows optical micrographs illustrating the temporal evolutions of the Plateau–Rayleigh instability for a liquid polystyrene film on a glass fibre (Haefner et al., 2015).

Using a lubrication approximation, the authors in Haefner et al. (2015) obtained a governing equation for the one-dimensional axisymmetric surface profile over time and compared with various experiments. In particular, they reported on the RI dynamics with two different boundary conditions on the liquid and fibre. The breakup of a liquid film coating a fiber into an array of droplets was simulated using a three-dimensional volume-of-fluid method by the authors in Mead-Hunter et al. (2012). They also compared the numerical results with experimental observations and existing theory. The instability of a liquid film coating a thin cylindrical fibre was investigated numerically and experimentally by González et al. (2010). They reported experimental results such as growth rates and dominant wavelengths of the interface. They also presented direct numerical simulations and compared with the experimental data.

In this work, we will use a phase-field method for the Rayleigh instability on a fibre and investigate the effects of the thickness of the liquid film and the fibre on the evolution dynamics. The phase-field method is popular in modeling two-phase fluid flows. For example, Bai et al. (2017) used a 3D phase-field model to simulate the droplet formation process in a flow-focusing device. There are other numerical methods for multiphase fluid flows such as the level-set method (Rodríguez, 2017) and the volume-of-fluid method (Müller et al., 2016).

The outline of the paper is as follows. The phase-field model in cylindrical coordinates is presented in Section 2. The numerical solution is given in Section 3. The proposed numerical schemes are tested in Section 4. Finally, conclusions are derived in Section 5.

2. Axisymmetric Navier–Stokes–Cahn–Hilliard system

We consider the two-phase fluid consisting of two components, fluid 1 and fluid 2, on a solid fibre. We denote by $\phi$ the composition difference of the mixture of two fluids. The phase-field $\phi$ is a normalized concentration and its value is equal to $+1$ and $-1$ when the two phases are at mutual equilibrium. In this study, we focus on density matched case. The axisymmetric Navier–Stokes–Cahn–Hilliard system (Kim, 2005b) is

$$\nabla \cdot \mathbf{u} = 0, \quad \rho(u_t + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \nabla \cdot \left[ \eta(\phi)(\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right] + \mathbf{S}F(\phi), \quad \phi_t + \nabla \cdot (\phi \mathbf{u}) = M \Delta \mu, \tag{1}$$

where $\rho$ is the density, $u$ is the velocity vector, $p$ is the pressure, $\eta$ is the viscosity, $\mathbf{S}$ is the stress tensor, $\phi$ is the phase-field, $F(\phi)$ is the free energy, and $\mu$ is the chemical potential.

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μ = αφ³ − βφ − κΔφ, \hspace{1cm} (4) 

where \( \mathbf{u} \) is the velocity, \( \rho \) is the density, \( p \) the pressure, and \( \eta(\phi) = \eta_1 (1 + \phi)/2 + \eta_2 (1 - \phi)/2 \) is the variable viscosity, where \( \eta_1 \) and \( \eta_2 \) are viscosity coefficients of fluid 1 and 2, respectively. The surface tension force \( \text{Kim, 2005a) is} \)

\[
\text{SF}(\phi) = \frac{3\sqrt{2}\sigma \epsilon}{4} \mathbf{\nabla} \cdot \left( \frac{\mathbf{\nabla} \phi}{|\mathbf{\nabla} \phi|} \right) |\mathbf{\nabla} \phi| \phi, \hspace{1cm} (5)
\]

where \( \sigma \) is the interfacial tension coefficient and \( \epsilon \) is the small positive number related to interfacial transition thickness. Other thermodynamically consistent surface tension force, i.e., the Korteweg force can be found in \( \text{Kim (2005a) and Lamorgese et al. (2017),} \)

\[
\mu = \phi^3 - \phi - \epsilon^2 \Delta \phi, \hspace{1cm} (9)
\]

where we set \( \alpha = 1, \beta = 1, \kappa = \epsilon^2 \) and the Reynolds, Weber, and Peclet numbers are given by \( R_e = \rho u L z/\eta c, \) \( W_e = \rho L u^2 / \sigma c, \) and \( P_e = U L z / (M c) \) using characteristic values, respectively. More details about the nondimensionalization can be found in \( \text{Kim (2005b) and} \)

\[
\text{Lee et al. (2011),} \text{ Because we are interested in axisymmetric Navier–Stokes–Cahn–Hilliard system for the cylindrical viscous liquid thread on a solid fibre, we rewrite Eqs. (6)–(9) in axisymmetric form:} \]

\[
\begin{align*}
\frac{1}{r} (ru)_r + w_z &= 0, \hspace{1cm} (10) \\
u_t + uu_r + wu_z &= -p_r + \frac{SF}{We} \\
\quad + \frac{1}{Re} \left( \frac{1}{r} (r(2\eta u_r))_r + (\eta(w_r + u_z))_z - \frac{2\eta u}{r^2} \right). \hspace{1cm} (11)
\end{align*}
\]

where \( u = u(r, z) \) and \( w = w(r, z) \) are the radial and the axial velocities, respectively. The subscript index is the differentiation with respect to that index.

### 3. Numerical solution

Let us consider a two-dimensional axisymmetric computational domain \( \Omega = \{ (r, z) : R_1 < r < R_2, \ 0 < z < H \} \). We discretize the domain with a uniform mesh spacing \( h \). The center of each cell is positioned at \( (r_i, z_k) = (R_1 + (i-0.5)h, k-0.5)h \) for \( i = 1, \ldots, N_r \) and \( k = 1, \ldots, N_z \), where \( N_r \) and \( N_z \) are the numbers of cells in \( r \) and \( z \)-directions, respectively. The cell vertices are located at \( (r_{i+\frac{1}{2}}, z_{k+\frac{1}{2}}) = (R_1 + ih, kh) \). Given \( \mathbf{u}^n = (u^n, w^n) \) and \( \phi^n \), we want to find \( \mathbf{u}^{n+1} = (u^{n+1}, w^{n+1}) \) and \( \rho^{n+1} \) which solve the following discrete Eqs. (10)–(12):

\[
\frac{1}{r} (ru^{n+1})_r + w^{n+1}_z = 0, \hspace{1cm} (15)
\]

Fig. 1. Plateau–Rayleigh instability for a liquid polystyrene film on a glass fibre. Adapted from Haehner et al. (2015) with permission from Nature Publishing Group.
\[
\frac{u^{n+1} - u^n}{\Delta t} = -(u_{ir} + w_{ir})^n - \frac{SF}{We} \frac{n}{r^2} + \frac{1}{Re} \left( \frac{1}{r} (r (2 \eta w_r)_r) + (\eta (w_r + u_z)_z) - \frac{2 \eta w_r}{r^2} \right) + \frac{S}{We} \left( \frac{2 \eta w_r}{r^2} \right).
\]

Fig. 4. Temporal evolution of a thread coating a fibre: (a) \(R_0 = 0.4\), (b) \(R_0 = 0.5\), and (c) \(R_0 = 0.6\). The rows from top to bottom are at \(t = 0\), 0.2602, 0.4241, 0.4723, and 0.5687.

To solve Eqs. (15)–(17), we use the projection method (Chorin, 1997). First, we solve an intermediate velocity field \(\tilde{u} = (\tilde{u}, w)\):

\[
\begin{align*}
\tilde{u}_{i+\frac{1}{2},k}^{n+1} &= u_{i+\frac{1}{2},k}^n - \Delta t (u_{ir} + w_{ir})_{i+\frac{1}{2},k}^n + \Delta t \frac{SF}{We} \frac{n}{r^2} + \Delta t \frac{S}{We} \left( \frac{2 \eta w_r}{r^2} \right), \\
\tilde{w}_{i+\frac{1}{2},k}^{n+1} &= w_{i+\frac{1}{2},k}^n + \frac{1}{h^2} \left( \frac{2 \eta w_r}{r^2} \right).
\end{align*}
\]

The values \(\tilde{u}_{i+\frac{1}{2},k}^n\) and \(\tilde{w}_{i+\frac{1}{2},k}^n\) are defined by the upwind procedure:

\[
\begin{align*}
\tilde{u}_{i+\frac{1}{2},k}^n &= \begin{cases} 
\frac{u_{i+\frac{1}{2},k}^n - u_{i-\frac{1}{2},k}^n}{h} & \text{if } u_{i+\frac{1}{2},k}^n > 0 \\
\frac{u_{i+\frac{1}{2},k}^n - u_{i-\frac{1}{2},k}^n}{h} & \text{otherwise},
\end{cases} \\
\tilde{w}_{i+\frac{1}{2},k}^n &= \begin{cases} 
\frac{w_{i+\frac{1}{2},k}^n - w_{i-\frac{1}{2},k}^n}{h} & \text{if } w_{i+\frac{1}{2},k}^n > 0 \\
\frac{w_{i+\frac{1}{2},k}^n - w_{i-\frac{1}{2},k}^n}{h} & \text{otherwise},
\end{cases}
\end{align*}
\]

The other quantities are similarly defined. At \(z = 0\) and \(z = H\), symmetric boundary condition is applied. At \(r = R_1\) and \(r = R_2\), no-slip boundary condition is used. After nondimensionalization, the surface tension term becomes

\[
\text{SF} = -\frac{3\sqrt{2} \epsilon}{4} \nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right) |\nabla \phi|.
\]

Let the normal vector at \((r_{i+\frac{1}{2},k+\frac{1}{2}})\) be given by

\[
\begin{align*}
n_{i+\frac{1}{2},k+\frac{1}{2}} &= (n_{i+\frac{1}{2},k+\frac{1}{2}}, n_{i+\frac{1}{2},k+\frac{1}{2}}) \\
&= \left( \frac{\Phi_{i+1,k+1} - \Phi_{i,k+1}}{2h}, \frac{\Phi_{i,k+1} - \Phi_{i+1,k}}{2h} \right).
\end{align*}
\]

Then, \(\nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right)\) is approximated by

\[
\nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right)_{i+\frac{1}{2},k+\frac{1}{2}} = \begin{cases} 
\frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} + \frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} + \frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} \\
\frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} - \frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} - \frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} \\
\frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} + \frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} + \frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} \\
\frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} - \frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|} - \frac{f_{i+\frac{1}{2},k+\frac{1}{2}}}{|n_{i+\frac{1}{2},k+\frac{1}{2}}|}.
\end{cases}
\]
To avoid division by very small numbers or by zero, we set $\nabla_d$: 
\[ \left( \frac{\nabla \phi}{\nabla \varphi} \right)_k = \begin{cases} \frac{1}{6} & \text{if } |n_i \cdot \frac{1}{2} + n_{i+1} \cdot \frac{1}{2} - n_{i+1} \cdot \frac{1}{2} + n_{i} \cdot \frac{1}{2} - n_{i} \cdot \frac{1}{2} | < 1.0 \times 10^{-12}, \end{cases} \]
which implies the surface tension force is localized in the neighborhood of the interface. The cell-centered normal is $\nabla_d \phi_k = (n_{i+1/2} - n_i + n_{i+1/2} - n_{i+1})/4$. When we need surface tension values at edges, we take the average of cell centered values. Next, we solve the following equations for the pressure field:
\[
\frac{u^{n+1} - \bar{u}}{\Delta t} = -\nabla_d \rho_{n+1},
\]
where
\[
\nabla_d \cdot u^{n+1} = 0,
\]
and
\[
\nabla_d \rho_{n+1} = \left( \frac{p_{i+1,k} - p_{i,k}}{h}, \frac{p_{i,k+1} - p_{i,k}}{h} \right).
\]
Note that the first and the second terms of the pressure gradient are stored at $(t_{i+1/2}, z_k)$ and $(t, z_{k+1})$, respectively. Taking the divergence operator to \Eqref{18} and using \Eqref{19}, we obtain the Poisson equation.
\[
\Delta_d \rho_{n+1} = \frac{\nabla_d \cdot \bar{u}}{\Delta t},
\]
where
\[
\nabla_d \rho_{n+1} = \frac{r_{i+1/2}(p_{i+1,k} - p_{i,k}) - r_{i-1/2}(p_{i,k} - p_{i-1,k})}{r_i h^2} + \frac{(p_{i,k+1} - p_{i,k}) - (p_{i,k} - p_{i-1,k})}{h^2},
\]
and
\[
\nabla_d \cdot \bar{u}_{n+1} = \frac{r_{i+1/2}\bar{u}_{i+1/2} - r_{i-1/2}\bar{u}_{i-1/2} + \bar{w}_{i+1/2} - \bar{w}_{i-1/2}}{h}.
\]
We solve \Eqref{20} by using a multigrid method (Trottenberg et al., 2001) and the divergence-free velocity is defined by
\[
u^{n+1} = \frac{\bar{u}}{\Delta t} \nabla_d \rho_{n+1}, \quad \text{i.e.,}
\]
\[
\nu_{i+1/2}^{n+1} = \bar{u}_{i+1/2} - \frac{\Delta t}{h} (p_{i+1,k} - p_{i,k}),
\]
\[
w_{i+1,k}^{n+1} = \bar{w}_{i+1,k} - \frac{\Delta t}{h} (p_{i,k+1} - p_{i,k}).
\]
We use a nonlinear gradient stable scheme (Eyre, 1998) for the axisymmetric Cahn–Hilliard equation.
\[
\bar{\omega}^{n+1} = \phi^n - \frac{r_{i+1/2}(\phi^n u^n)_{i-1/2} - r_{i-1/2}(\phi^n u^n)_{i+1/2}}{r_i h},
\]
\[
\frac{\phi^n}{h} - \frac{(\phi^n)_{i+1/2} - (\phi^n)_{i-1/2}}{h} - \frac{1}{\beta \eta} \left( \frac{r_{i+1/2}(\mu_{i+1,k}^{n+1} - \mu_{i,k}^{n+1}) - r_{i-1/2}(\mu_{i,k}^{n+1} - \mu_{i-1,k}^{n+1})}{r_i h^2} \right),
\]
\[
\mu_{i+1,k}^{n+1} = \phi_{i,k}^{n+1} - \frac{(\phi_{i+1/2,k}^{n+1})^3 - \phi_{i,k}^n}{r_{i+1/2,k}} - \frac{\phi_{i+1,k}^{n+1} - \phi_{i,k}^{n+1}}{r_i h^2},
\]
\[
\phi_{i,k}^{n+1} = \phi_{i,k}^n - \frac{1}{\beta \eta} \left( \frac{r_{i+1/2}(\phi_{i+1/2,k}^{n+1} - \phi_{i,k}^{n+1}) - r_{i-1/2}(\phi_{i,k}^{n+1} - \phi_{i-1/2,k}^{n+1})}{r_i h^2} \right).}
\]
We apply a nonlinear multigrid method (Kim, 2005b; Trottenberg et al., 2001) to solve the discrete system of \Eqref{21} and \Eqref{22}.

### 4. Numerical simulations

Before we start, we define the interfacial length parameter $\epsilon_m$ as follows:
\[
\epsilon_m = \frac{\sqrt{2} \tan^{-1}(0.9)}{2 \eta}
\]
which implies that we have approximately $\epsilon_m$ transition layer width (Kim, 2012). For all tests, we use $\epsilon = \epsilon_m$ for some integer $m$ and $90^\circ$ contact angle boundary condition, unless otherwise specified.

We consider a perturbed cylindrical thread of a viscous fluid coating a fibre, the viscosity and density of which are denoted by $\eta$ and $\rho$, respectively, in another viscous fluid of viscosity $\eta_o$ and density $\rho_o$. In the unperturbed profile, the interface has a cylindrical shape with radius $R_0$, see \Figref{2}. Typically, the characteristic values of length, viscosity, and density scales are the diameter of a fibre $R_c = 2R_1 = 110\mu m$, $R_1 = 11 - 23$ poise, and $\rho_c = 0.96\text{ gcm}^{-3}$, respectively, and $0.7L_c < R_0 < 2.125L_c$ (González et al., 2010). The characteristic velocity is defined as $U_k = \sqrt{\eta / (\rho_0 L_c)}$ because the flow under consideration is surface tension driven flow.

\Figref{3} shows temporal evolution of a thread coating a fibre. The initial phase field and velocity fields are given by
\[
\phi(r, z, 0) = \tanh \left( \frac{R_0 - r}{\alpha_0 \cos(z)} \right),
\]
\[
u(r, z, 0) = w(r, z, 0) = 0
\]
on a domain, $\Omega = \{(r, z)|R_1 \leq r \leq R_1 + \pi \text{ and } 0 \leq z \leq 2\pi\}$. We use the parameters: $R_0 = 0.5$, $R_1 = 0.2$, $\alpha_0 = 0.05$, $h = \pi / 128$, $\Delta t = 0.2h^2$, $\epsilon = \epsilon_d$, $Re = 0.16$, $We = 0.002$, $Pe = 1/\epsilon$, and viscosity ratio $\beta = \eta_0/\eta_1 = 0$. In the following tests, unless otherwise specified, we use \Eqref{23} and \Eqref{24} as an initial condition and the above parameter values.

#### 4.1. Effect of $R_0$

We investigate the effect of $R_0$ on the thread dynamics. The initial conditions are \Eqref{23} and \Eqref{24}. We fix $R_1 = 0.2$.

\Figref{4} shows the temporal evolution of a thread coating a fibre with $R_0 = 0.4$, $R_0 = 0.5$, and $R_0 = 0.6$, respectively. As $R_0$ increases, the size of the satellite droplet decreases.

#### 4.2. Effect of $R_1$

We investigate the effect of $R_1$ on the thread dynamics. The initial conditions are \Eqref{23} and \Eqref{24}. We fix $R_0 = 0.6$. \Figref{5} shows the temporal evolution of a thread coating a fibre with $R_1 = 0.2$, $R_1 = 0.3$, and $R_1 = 0.4$, respectively. As $R_1$ increases, the size of the satellite droplet decreases.

Next, we highlight the effect of thickness of the fibre $R_1$ on the breakup of the coating thread. \Figref{6} shows the temporal evolution of a thread coating a fibre with $R_1 = 0.4$ and (b) $R_1 = 0.8$, respectively. Here, $R_0 = 0.95$, $Re = 1$ and $We = 0.01$ are used. In the absence of the fibre, if the wave-length of the liquid column is greater than the circumference of the cylinder, then sinusoidal perturbation is unstable (Tomotika, 1935). However, by comparing \Figref{6} and (b), we can find that the thick fibre significantly delays the process of Rayleigh instability, i.e., it takes a long time before the liquid undergoes pinch-off.

#### 4.3. Effect of contact angle between solid fibre and liquid

We consider the effect of the surface tension between the solid fibre and the liquid on the interfacial dynamics, which is equivalently the effect of contact angle between the solid fibre and the liquid. \Figref{7} shows the schematic illustration of the contact angle.
Fig. 5. Temporal evolution of a thread coating a fibre: (a) $R_1 = 0.2$, (b) $R_1 = 0.3$, and (c) $R_1 = 0.4$. The rows from top to bottom are at $t = 0$, 2.1144, 2.6566, 3.3673, and 8.0781.

Fig. 6. Temporal evolution of a thread coating a fibre: (a) $R_1 = 0.4$ and (b) $R_1 = 0.8$. Here, $R_0 = 0.95$ is used. The rows from top to bottom are at $t = 0$, 14.3369, 19.1561, 20.6018, and 29.9992.

The contact angle boundary condition on the solid fibre is given as

$$\mathbf{n} \cdot \nabla \phi(r, z, t) = -\frac{G'(\phi(r, z, t))}{\epsilon^2}, \quad (25)$$

where $\mathbf{n}$ is an outer unit normal vector to $\partial \Omega$ and $G(\phi) = \epsilon (\phi^3 - 3\phi) \cos \theta/(3\sqrt{2})$ is the specific wall free energy with the contact angle $\theta$, see Lee and Kim (2011) and references therein for more details about the contact angle boundary condition. At $r = R_1$, the discrete form of Eq. (25) can be written as

$$-\phi_r = -\frac{\phi_{1k} - \phi_{0k}}{h} = -\frac{(\phi_{1k}^2 - 1) \cos \theta}{\sqrt{2} \epsilon}, \quad \text{for } k = 1, \cdots, N_z. \quad (26)$$
Then, we can obtain the discrete form of contact angle boundary condition from Eq. (26)

\[
\phi_{bk} = \phi_{bk} - \frac{h(\phi_{bk}^2 - 1) \cos \theta}{\sqrt{2e}},
\]

where \(\phi_{bk} = (3\phi_{1k} - \phi_{2k})/2\). Next, we take the contact angles 30°, 60°, 90°, 120°, and 150° to investigate the effect of contact angle between the liquid and the solid fibre. Here, \(R_0 = 0.95\) and \(R_1 = 0.4\) are used. From Fig. 8, we can find that the different contact angles between liquid and fibre cause the different temporal evolutions of a liquid thread. As the contact angle increases, it shows the fast dynamics.

5. Conclusion

In this article, we presented a phase-field method for Rayleigh instability on a fibre. The Navier–Stokes–Cahn–Hilliard system was used to model axisymmetric immiscible two-phase flow with surface tension on a fibre. For the numerical solutions, the projection method and the nonlinearly stable splitting method were employed. We presented computational experiments with various thicknesses of liquid thread and fibre. Unlike a liquid column, the evolutionary dynamics of a liquid layer on a fibre depended on the thickness of the fibre. The numerical results indicated that the size of the satellite droplet decreases as the thicknesses of the thread and fibre increase. In upcoming work, we will investigate the effect of the gravitational force on the fluid dynamics on a fibre.

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