Physically-Based Droplet Interaction: Supplementary Material

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As this work relies an existing model from another field, for completeness, we give the main details on its derivation in this document.

1 Collision Threshold Derivation

We use the collision thresholds originally derived and validated by Ashgriz and Poo [1990]. These were developed to offer physically-accurate, energy-based prediction of the outcome type of a droplet collision based on the colliding state of the pair of droplets. We consider the collision between the pair of spherical droplets i, j with positions $\mathbf{x}_i, \mathbf{x}_j$ velocities $\mathbf{u}_i, \mathbf{u}_j$ and radii $r_i > r_j$.

1.1 Stretching Separation

Stretching separation is considered to arise for collisions in which the stretching kinetic energy in the collision is greater than the surface energy of the ligament that forms between the colliding droplets.

Assuming that the collision is such that only a portion of the droplet masses come into contact, we define the volume of interaction of droplet i as $\phi_i V_i$, for V_i the volume of the sphere of radius r_i, centre $\mathbf{x}_i$, cut by the planes parallel to $\mathbf{u}_{ij}$ and tangential to edge of the other droplet sphere, j (Fig. 4 - main paper), and similarly for droplet j.

In Ashgriz and Poo [1990], the following equations for ϕ_i, ϕ_j are given:

$$\phi_i = \begin{cases} 1 - \frac{(2-\tau)^2(1+\tau)}{4}, & \text{if } h > r_i. \\ \frac{\tau^2(3-\tau)}{4}, & \text{otherwise.} \end{cases} \tag{1}$$

$$\phi_j = \begin{cases} 1 - \frac{(2\delta-\tau)^2(\delta+\tau)}{4\delta^3}, & \text{if } h > r_j. \\ \frac{\tau^2(3\delta-\tau)}{4\delta^3}, & \text{otherwise.} \end{cases} \tag{2}$$

where $h = (1 - X)(r_1 + r_2)$ and $\tau = (1 - X)(1 + \delta)$. In the main paper, we note that these equations are not valid for the case of a fully overlapped smaller droplet $h > 2r_j$ (where we should have $\phi_j = 1$) and instead suggest calculating these with geometric equations for segments and caps in these cases.

Now, assuming that the remaining non-interacting portions of the droplets continue along their initial trajectory, we calculate the kinetic stretching energy in the entire collision as:

$$\begin{aligned}
\mathbf{E}_{stretch} &= \text{non-interacting KE} + \text{interacting KE} \\
&= \frac{1}{2}\rho[(V_i - V_{i,I})||\mathbf{U}_i||^2 + (V_j - V_{j,I})||\mathbf{U}_j||^2] + \frac{1}{2}\rho[V_{i,I}(\mathbf{U}_i X)^2 + V_{j,I}(\mathbf{u}_j X)^2] \\
&= \frac{1}{2}\rho[(1-\phi_i)V_i||\mathbf{U}_i||^2 + (1-\phi_j)V_j||\mathbf{U}_j||^2] + \frac{1}{2}\rho X^2[V_{i,I}||\mathbf{U}_i||^2 + V_{j,I}||\mathbf{U}_j||^2] \\
&= \frac{1}{2}\rho||\mathbf{U}_{ij}||^2 V_i \left(\frac{\delta^3}{(1+\delta^3)^2}\right)[(1+\delta^3) - (1-X^2)(\phi_j + \delta^3\phi_i)]
\end{aligned} \tag{3}$$

Note that the above equation, as described in Ashgriz and Poo [1990], velocity is formulated in mass-centre coordinates (corrected by Ko and Ryou [2005]), so uses:

$$\mathbf{U}_i = \frac{-\delta^3\mathbf{u}_{ij}}{(1+\delta^3)} \tag{4}$$

$$\mathbf{U}_j = \frac{\mathbf{u}_{ij}}{(1+\delta^3)} \tag{5}$$

but that any use of the relative velocity $\mathbf{U}_{ij}$ remains equal to the usual form, $\mathbf{U}_{ij} = \frac{(1+\delta^3)\mathbf{u}_{ij}}{1+\delta^3} = \mathbf{u}_{ij}$.

The surface energy that opposes this stretching is that of the nominal ligament created from the interacting volume, given by the surface energy associated with a cylinder of height h and volume $V_{interact} = V_{interact,i} + V_{interact,j}$:

$$\begin{aligned}
\mathbf{E}_{surface} &= 2\sigma[\pi h V_{interact}]^{\frac{1}{2}} \\
&= 2\sigma[\pi h(V_{interact,i} + V_{interact,j})]^{\frac{1}{2}} \\
&= 2\sigma[\pi V_i r_i \tau(\phi_i + \delta^3\phi_j)]^{\frac{1}{2}}
\end{aligned} \tag{6}$$

Then if $\mathbf{E}_{stretch} > \mathbf{E}_{surface}$ the collision results in stretching separation.

Considering the equality of the above equation and then rearranging allows definition of a threshold on We as $\mathrm{We}_{stretch}$:

$$\mathrm{We}_{stretch} = \frac{4(1+\delta^3)^2[3(1+\delta)(1-X)(\delta^3\phi_j + \phi_i)]^{\frac{1}{2}}}{\delta^2[(1+\delta^3) - (1-X^2)(\phi_j + \delta^3\phi_i)]} \tag{7}$$

such that the stretching separation threshold is surpassed if $\mathrm{We} > \mathrm{We}_{stretch}$.

1.2 Reflexive Separation

For head-on collisions, we check for reflexive separation in a similar way to that of stretching separation. This outcome is said to arise due to a combination of the incident kinetic energies working in opposing directions, and the internal flows induced due to the difference between the colliding droplet surface energies and the nominal coalesced droplet surface energy.

The kinetic energy term is that of the portions of the droplets which directly oppose each other, given by:

$$\mathbf{E}_{counter} = \frac{1}{2}\rho(V_{i,P}||\mathbf{U}_i||^2 + V_{j,P}||\mathbf{U}_j||^2) \tag{8}$$

where the volume $V_{k,P}$ is the volume of the prolate regions of the incident droplets, defined in terms of X by:

$$V_{i,P} = \frac{4}{3}\pi r_i^3(1-\xi)^2(1-\xi^2)^{\frac{1}{2}} \tag{9}$$

$$V_{j,P} = \frac{4}{3}\pi r_i^3(\delta-\xi)^2(\delta^2-\xi^2)^{\frac{1}{2}} \tag{10}$$

where $\xi = \frac{1}{2}X(1+\delta)$. Then the excess surface energy is given by:

$$\mathbf{E}_{excess} = 4\sigma\pi r_i^2[(1+\delta^2)-(1+\delta)^{\frac{2}{3}}] \tag{11}$$

Finally, the remaining portions of droplets try to stretch the combined mass, which reduces the reflexive energy above and so we also include the following stretching energy term:

$$\mathbf{E}_{stretch} = \frac{1}{2}\rho[(V_i - V_{i,P})||\mathbf{U}_i||^2 + (V_j - V_{j,P})||\mathbf{U}_j||^2] \tag{12}$$

The effective reflexive energy is therefore given by:

$$\mathbf{E}_{reflex} = \mathbf{E}_{counter} + \mathbf{E}_{excess} - \mathbf{E}_{stretch} \tag{13}$$

which can be rearranged to:

$$\mathbf{E}_{reflex} = 4\sigma\pi r_i^2\left[(1+\delta^2)-(1+\delta^3)^{\frac{2}{3}} + \frac{We}{12\delta(1+\delta^3)^2}(\delta^6\eta_i+\eta_j)\right] \tag{14}$$

where

$$\eta_i = 2(1-\xi)^2(1-\xi)^{\frac{1}{2}} - 1 \tag{15}$$

$$\eta_j = 2(\delta-\xi)^2(\delta^2-\xi^2)^{\frac{1}{2}} - \delta^3 \tag{16}$$

Reflexive separation is then said to occur when this energy exceeds 75% of the surface energy of the nominal coalesced mass $\mathbf{E}_{surface,k} = 4\sigma\pi(r_i^3 + r_j^3)^{\frac{2}{3}}$, i.e. when $\mathbf{E}_{reflex} > 0.75\mathbf{E}_{surface,k}$.

Using these formulations for $\mathbf{E}_{reflex}$ and $\mathbf{E}_{surface,k}$ taking the threshold of the above inequality and rearranging for We gives:

$$We_{reflex} = \frac{3[7(1+\delta^3)^{\frac{2}{3}} - 4(1+\delta^2)]\delta(1+\delta^3)^2}{(\delta^6\eta_i+\eta_j)} \tag{17}$$

and thus a collision with $We > We_{reflex}$ will exhibit reflexive separation.

References

N. Ashgriz and J.Y. Poo. 1990. Coalescence and separation in binary collisions of liquid drops. *Journal of Fluid Mechanics* 221 (1990), 183–204.

G.H. Ko and H.S. Ryou. 2005. Modeling of droplet collision-induced breakup process. *International Journal of Multiphase Flow* 31, 6 (2005), 723–738.