**Supplementary material: Progressive evolution of viscous dissipation mechanism from the macroscale to the nanoscale**

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**Content:**

This supplementary material includes (1) the statements of interactions of nitrogen particles (n-n) and between nitrogen and other particles (n-w and n-s) with corresponding parameters (**Table S1**), (2) the description of data used in this work (**Table S2**), (3) the validation of *C*bulk=0.4 by direct measurement in simulations (**Figure S1**), and (4) a reference list for this supplementary material.

**The statements of interactions of nitrogen particles (n-n) and between nitrogen and other particles (n-w and n-s)**

The interactions of nitrogen particles (n-n) and between nitrogen and other particles (n-w and n-s) is simulated by the DPD method; this DPD-MDPD coupled simulation system for incorporating the effect of ambient gas has been attested in previous studies (Lin *et al*. 2021a, 2021b). The DPD interaction can be simply achieved by setting *B*=0 and using a positive value of *A* based on the MDPD interaction (Eqs. (3-5)), i.e.,

|  |  |  |
| --- | --- | --- |
|  |  | (S1) |
|  |   | (S2) |
|  |  | (S3) |

Here, *ω*D(*rij*)=*ω*R(*rij*)2=*ω*c(*rij*)2=(1-*rij*/*r*dpd)2. The parameters used for n-n, n-w, and n-s interactions by DPD method are shown in **Table S1**.

**Table S1.** The parameters of gas particles.

|  |  |  |
| --- | --- | --- |
| Parameter | Symbol | Value |
| DPD coefficient | *A*n-n,dpd, *A*n-w,dpd, *A*n-s,dpd | 8 |
| System temperature | *k*B*T* | 1 |
| DPD dissipation parameter | *γ*dpd | 24 |
| DPD interaction range | *r*dpd | 1 |
| Time step | Δ*t* | 0.01 |

**Table S2.** The description of data used in this work.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | *Oh* | *θ* | Source | Used for |
| Series 1 (Exp.) | 0.002 | 162° | Antonini, Amirfazli & Marengo (2012) | Test |
| Series 2 (Exp.) | 0.003 | 90° | Stow & Hadfield (1981) | Test |
| Series 3 (Exp.) | 0.21 | 163° | Abolghasemibizaki *et al.* (2019) | Test |
| Series 4 (Exp.) | 0.56 | 120° | Du, Zhang & Min (2021) | Fitting |
| Series 5 (Exp.) | 1.05 | 90°**\*** | Clanet *et al*. (2004) | Test |
| Series 6 (MDPD) | 0.21 | 100° | This work | Test |
| Series 7 (MDPD) | 0.21 | 109° | This work | Test |
| Series 8 (MDPD) | 0.21 | 125° | This work | Fitting |
| Series 9 (MDPD) | 0.21 | 137° | This work | Test |
| Series 10 (MDPD) | 0.21 | 147° | This work | Test |
| Series 11 (MDPD) | 0.21 | 164° | This work | Test |
| Series 12 (MDPD) | 0.096 | 125° | This work | Test |
| Series 13 (MD) | 0.35 | 125° | Wang *et al*. (2020), Wang *et al*. (2022) | Test |
| Series 14 (MD) | 0.35 | 148° | Wang *et al*. (2022) | Fitting |
| Series 15 (MD) | 0.35 | 165° | This work | Test |
| Series 16 (MD) | 0.48 | 180° | Zhang *et al*. (2014) | Test |

**\***This series of data is from silicone oil droplets impacting a smooth plastic surface. Here, *θ*=90° is used for calculating in the proposed model.

**The validation of *C*bulk=0.4 by direct measurement in simulations**

In this validation, the velocity fields extracted from simulations are used to directly prove the fitted value of *C*bulk. In our manuscript, the final expression of bulk viscous dissipation based on the equivalent *V*bulk, i.e., Eq. (20), is expressed as,

|  |  |  |
| --- | --- | --- |
|  |  | (S4) |

Here, *V*bulk in *C*bulk(=*V*bulk/*V*0) is an equivalent velocity characterising the strength of extensional flow, which cannot be directly extracted from simulations. Simulations can only capture time-varying *V*bulk,*t* (or *β*-varying *V*bulk,*β* for the convenience of integration of *β* in Eq. (S4)) satisfying the extensional flow assumption during spreading. Considering *β*-varying *V*bulk,*β*, Eq. (S4) should be expressed as,

|  |  |  |
| --- | --- | --- |
|  |  | (S5) |

By equaling Eq. (S4) and Eq. (S5), it can be obtained as,

|  |  |  |
| --- | --- | --- |
|  |  | (S6) |

Equation (S6) can be simplified as,

|  |  |  |
| --- | --- | --- |
|  |  | (S7) |

By substituting the measured results of *C*bulk,*β* into Eq. (S7), the measured value of *C*bulk can be obtained. If this measured *C*bulk matches the fitted result (*C*bulk =0.4), it further convinces the validity of *C*bulk=0.4. **Figure S1(a-c)** show the curves of *C*bulk,*β*2/*β*2 as a function of *β* for nanodroplets impacting surfaces with *θ*=148° at *We*=30.6, 45.7, and 73.9, obtaining the integrated values of *C*bulk,*β*2/*β*2 as 0.059, 0.067, and 0.082, respectively. Meanwhile, the maximum spreading factors for these cases are measured as *β*max=1.54, 1.74, and 2.02. Substituting these measured results into Eq. (S7), yielding measured *C*bulk of 0.410, 0.397 and 0.403, respectively, as shown in **Fig. S1(d)**. These measured *C*bulk are consistent with the fitted result, thus proving the validity of *C*bulk=0.4.



**Figure S1**. Values of *C*bulk,*β*2/*β*2 varying with *β* for impacting nanodroplets (*Oh*=0.35) at *We*=(a) 30.6, (b) 45.7, and (c) 73.9 on surfaces with *θ*=148°. These cases are from data Series 14. The values of *V*bulk,*β* to calculate *C*bulk,*β*(=*V*bulk,*β*/*V*0) are obtained by inversely solving *Vr*=*r*/*RV*bulk,*β* through velocity fields captured from simulations at different spreading factors. (d) Comparison between the measured values of *C*bulk for different cases and the fitted value of *C*bulk=0.4.

**References for this supplementary material:**

ABOLGHASEMIBIZAKI, M., DILMAGHANI, N., MOHAMMADI, R. & CASTANO, C.E. 2019 Viscous droplet impact on nonwettable textured surfaces. *Langmuir* **35**, 10752-10761.

ANTONINI, C., AMIRFAZLI, A. & MARENGO, M. 2012 Drop impact and wettability: from hydrophilic to superhydrophobic surfaces. *Phys. Fluids* **24**, 102104.

CLANET, C., BÉGUIN, C., RICHARD, D. & QUÉRÉ, D. 2004 Maximal deformation of an impacting drop. *J. Fluid Mech*. **517**, 199-208.

DU, J., ZHANG, Y. & MIN, Q. 2021 Numerical investigations of the spreading and retraction dynamics of viscous droplets impact on solid surfaces. *Colloids Surf. A* **609**, 125649.

LIN, C., LI, Z., LU, L., CAI, S., MAXEY, M. & KARNIADAKIS, G. E. 2021a Operator learning for predicting multiscale bubble growth dynamics. *J Chem. Phys.* **154**, 104118.

LIN, C., MAXEY, M., LI, Z. & KARNIADAKIS, G. E. 2021b A seamless multiscale operator neural network for inferring bubble dynamics. *J. Fluid Mech.* **929**, A18.

STOW, C.D. & HADFIELD, M.G. 1981 An experimental investigation of fluid flow resulting from the impact of a water drop with an unyielding dry surface. *Proc. R. Soc. A Math. Phys. Eng. Sci.* **373**, 419-441.

WANG, Y.-B., WANG, Y.-F., GAO, S.-R., YANG, Y.-R., WANG, X.-D. & CHEN, M. 2020 Universal model for the maximum spreading factor of impacting nanodroplets: from hydrophilic to hydrophobic surfaces. *Langmuir* **36**, 9306-9316.

WANG, Y.-F., WANG, Y.-B., HE, X., ZHANG, B.-X., YANG, Y.-R., WANG, X.-D. & LEE, D.-J. 2022 Scaling laws of the maximum spreading factor for impact of nanodroplets on solid surfaces. *J. Fluid Mech*. **937**, A12.

ZHANG, R., FAROKHIRAD, S., LEE, T. & KOPLIK, J. 2014 Multiscale liquid drop impact on wettable and textured surfaces. *Phys. Fluids* **26**, 082003.