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**Author for correspondence:**

Francesco Picano  
e-mail: francesco.picano@unipd.it

## Supplementary Material of Modeling the direct virus exposure risk associated to respiratory events

Jietuo Wang<sup>1</sup>, Federico Dalla Barba<sup>2</sup>,  
Alessio Roccon<sup>3,4</sup>, Gaetano Sardina<sup>5</sup>,  
Alfredo Soldati<sup>3,4</sup> and Francesco Picano<sup>1,2</sup>

<sup>1</sup>Centro di Ateneo di Studi e Attività Spaziali - CISAS,  
University of Padova, Padova, 35131, Italy

<sup>2</sup>Department of Industrial Engineering, University of  
Padova, Padova, 35131, Italy

<sup>3</sup>Institute of Fluid Mechanics and Heat Transfer, TU  
Wien, Vienna, 1060, Austria

<sup>4</sup>DPIA, University of Udine, 33100, Udine, Italy

<sup>5</sup>Department of Mechanics and Maritime Sciences,  
Chalmers University of Technology, 41296,  
Gothenburg, Sweden

## Formula Derivation

The temporal evolution of the position, velocity, size and temperature of an evaporating droplet, whose size is smaller than the smallest scales of the turbulent carrier flow, can be described in the framework of the so-called *point-droplet approximation* [1]. In this framework, an evaporating droplet is modelled as a rigid point-wise sphere whose dynamics is described by the following Lagrangian equations [2, 3, 4, 5]:

$$\frac{du_d}{dt} = \frac{1}{f} \frac{\bar{u} - u_d}{\tau_d} + \frac{\rho_d - \bar{\rho}}{\rho_d} g, \quad f = \frac{1}{1 + 0.15 Re_d^{0.687}}, \quad (0.1)$$

$$\frac{dD_d^2}{dt} = -4 \frac{Sh}{\bar{S}c} \frac{\bar{\rho}}{\rho_d} \bar{\nu} H_m, \quad (0.2)$$

$$\frac{dT_d}{dt} = \frac{1}{3\tau_d} \left[ \frac{Nu}{\bar{P}r} \frac{\bar{c}_p}{c_d} (\bar{T} - T_d) - \frac{Sh}{\bar{S}c} \frac{\Delta H_v}{c_d} H_m \right], \quad (0.3)$$

where  $u_d$  is the droplet velocity,  $D_d$  is the droplet diameter, and  $T_d$  is the temperature of the droplet. The over-bar notation refers to Eulerian quantities, describing the carrier flow, evaluated at the instantaneous position of the point-droplet. Equation (0.1) is the one-dimensional governing equation of a sphere in viscous flow. The variable  $\bar{u}$  is the velocity of the moist airflow carrying the droplet evaluated at the position of the droplet itself and  $\bar{\rho}$  its density. Gravitational acceleration,  $g$ , and buoyancy forces are accounted for by the second right-hand side term of equation (0.1). The parameter  $\tau_d$  is called droplet relaxation time,  $\tau_d = \rho_d D_d^2 / (18\bar{\mu})$ , with  $\rho_d$  the water droplet density and  $\bar{\mu}$  the dynamic viscosity of the airflow. A factor  $f$  is used to account for droplet finite inertia, which is a function of the droplet Reynolds number,  $Re_d = \|\bar{u} - u_d\| D_d / \bar{\nu}$ , with  $\bar{\nu}$  the kinematic viscosity of the carrier flow. Equation (0.2) governs the evolution of the droplet diameter, whereas equation (0.3) describes the temporal evolution of the droplet temperature. The variable  $\bar{T}$  is the temperature of the moist air flow that carries the droplets. The parameters  $\bar{S}c = \bar{\nu} / D_{a,v}$  and  $\bar{P}r = \bar{\mu} \bar{c}_p / \bar{k}$  are the Schmidt and Prandtl numbers, respectively, with  $\bar{c}_p$  the isobaric specific heat capacity of the moist air flow, and  $\bar{k}$  its thermal conductivity. The parameter  $D_{g,v}$  is the mass diffusivity of water vapor into air, whereas  $c_d$  and  $\Delta H_v$  are the specific heat capacity of liquid droplet and its latent heat of vaporization, respectively. As  $(\bar{T} - T_d)$  is the forcing term for convective heat transfer, the term  $H_m$  drives the mass transfer rate:

$$H_m = \ln \left( \frac{1 - \bar{Y}_v}{1 - Y_{v,d}} \right), \quad (0.4)$$

with  $\bar{Y}_v(\bar{\chi}_v)$  the vapor mass fraction in the carrier flow evaluated at the droplet center and  $Y_{v,d}(\chi_{v,d})$  the mass fraction of a saturated gas-vapor mixture evaluated at the temperature of the droplet,  $T_d$ . The vapor mass fractions depend on the vapor molar fractions:

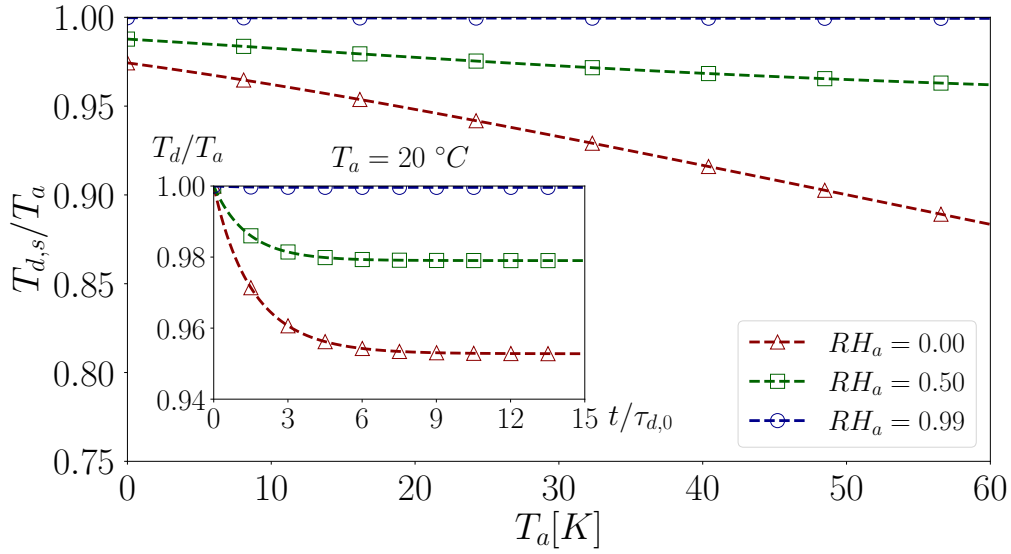
$$\bar{Y}_v = \frac{\bar{\chi}_v}{\bar{\chi}_v + (1 - \bar{\chi}_v) \frac{W_a}{W_d}}, \quad Y_{v,d} = \frac{\chi_{v,d}}{\chi_{v,d} + (1 - \chi_{v,d}) \frac{W_a}{W_d}}, \quad (0.5)$$

which, in turn, are related to the vapor pressure:

$$\bar{\chi}_v = \bar{R}H \frac{p_{sv}(\bar{T})}{p_a}, \quad \chi_{v,d} = 1.0 \frac{p_{sv}(T_d)}{p_a}, \quad (0.6)$$

where  $p_a$  is the ambient pressure,  $p_{sv}(\bar{T})$  the saturated vapor pressure evaluated at  $\bar{T}$ ,  $\bar{R}H$  the relative humidity of the moist carrier,  $W_a$  and  $W_d$  the molar weight of air and liquid water, respectively. The saturated vapour pressure depends on temperature and pressure and can be calculated by using the Clausius-Clapeyron equation. Finally, the Nusselt number,  $Nu$ , and Sherwood number,  $Sh$ , are correlated to the droplet Reynolds number via the Frössling correlations, see e.g. Wang et al. [6] for details.

Let consider an evaporating droplet in an environment with uniform thermodynamic properties,  $T_a$ ,  $p_a$ ,  $\rho_a$  and  $RH_a$  being the uniform ambient temperature, pressure, density and



**Figure 1.** Main panel: the ratio between the asymptotic droplet temperature,  $T_{d,s}$ , computed according to equation (0.11) and ambient temperature,  $T_a$ , versus ambient temperature itself for an isolated water droplet. Inset: temporal evolution of the temperature of an evaporating water droplet; the time is normalized by  $\tau_{d,0}$ , the initial relaxation time. Data are obtained by the numerical solution of equation (0.2) and equation (0.3).

relative humidity, respectively. Since  $H_m$  in equation (0.2) depends on the droplet temperature, ambient temperature and pressure, it can be assumed to be constant during evaporation. Under this assumption equation (0.2) can be integrated analytically:

$$D_d(t) = \sqrt{D_{d,0}^2 - kt}, \quad k = 4 \frac{\rho_a}{\rho_d} \frac{Sh}{Sc_a} \nu_a H_m(T_d, T_a, p_a, RH_a), \quad (0.7)$$

with  $D_{d,0}$  the droplet initial diameter and  $k$  a decay constant. When the effect of non-volatile matter is taken into account [7], one can estimate the droplet evaporation time as:

$$t_e = D_{d,0}^2 (1 - \psi^{2/3}) / k. \quad (0.8)$$

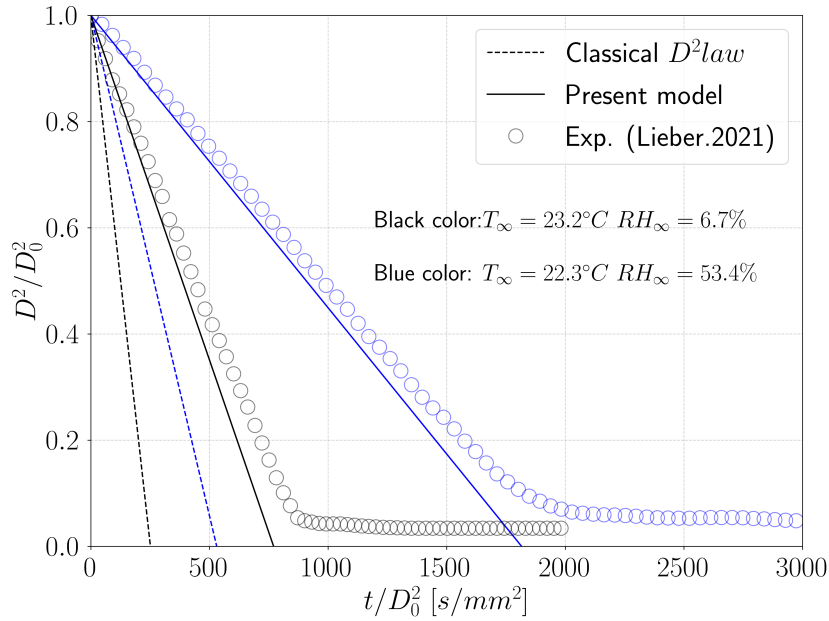
with  $\psi$  being the volume fraction of non-volatile matter inside each droplet. In the present model, assuming for simplicity  $\psi = 0$ , equation (0.8) can be rewritten as:

$$t_e = D_{d,0}^2 / k. \quad (0.9)$$

Equation (0.7) is historically referred to as  $\mathcal{D}^2$ -law since it predicts a linear temporal evolution of the square droplet diameter (surface), and it is used in the classical model of Wells, which implicitly assumed that the droplet temperature is fixed and equal to the initial one  $T_{d,0}$  during the whole vaporization process. Under this assumption the constant  $k$  is:

$$k = 4 \frac{\rho_a}{\rho_d} \frac{Sh}{Sc_a} \nu_a H_m(T_{d,0}, T_a, p_a, RH_a). \quad (0.10)$$

Nonetheless, this condition holds only for a short time of the order of few droplet relaxation times,  $\tau_d = \rho_d D_{d,0}^2 / (18\bar{\mu})$ , as can be seen in the inset of figure 1. The initial droplet temperature is equal to the environmental one,  $T_a$ ; nonetheless, after a time  $t \simeq 6\tau_{d,0}$ , the droplet temperature sets to an asymptotic value,  $T_{d,s}$ , which is lower than  $T_a$  depending on  $RH_a$ . Hence, the droplet temperature remains close to the ambient one only for  $t \simeq \tau_{d,0}$ , whereas, for the major part of the vaporization process, it keeps closer to an asymptotic temperature,  $T_{d,s}$ . By imposing  $dT_d/dt = 0$



**Figure 2.** Comparison of the decay of the square droplet diameter of saliva droplets predicted by the classical  $D^2$ -law model (dashed lines), the present revised  $D^2$ -law model (solid lines) and experimental benchmark data (symbols) from Lieber et al. [8]. Different environmental conditions are considered:  $T_\infty = 23.2^\circ\text{C}$   $RH_\infty = 6.7\%$  and  $T_\infty = 22.3^\circ\text{C}$   $RH_\infty = 53.4\%$ .

in equation (0.3), we obtain the following relation for the asymptotic temperature:

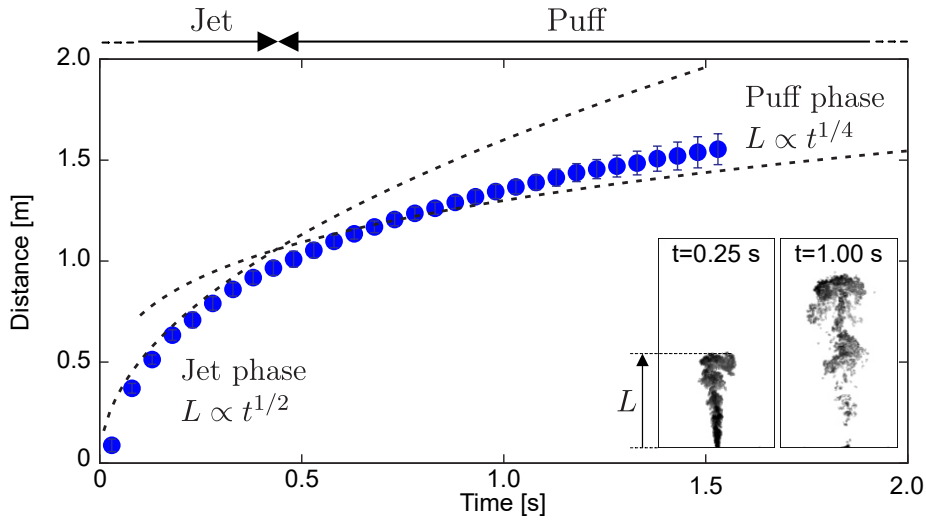
$$T_{d,s} + \frac{Pr_a}{Sc_a} \frac{Sh}{Nu} \frac{\Delta H_v}{c_{p,a}} H_m(T_a, p_a, RH_a, T_{d,s}) - T_a = 0, \quad (0.11)$$

$$H_m = \ln \left( \frac{1 - Y_v(T_a, p_a, RH_a)}{1 - Y_{v,d}(T_{d,s}, p_a)} \right), \quad (0.12)$$

which can be easily solved for  $T_{d,s}$ . The latter can be employed to compute a more accurate value of the decay constant,  $k$ :

$$k = \frac{\rho_a}{\rho_d} \frac{Sh}{Sc_a} \nu_a H_m(T_{d,s}, T_a, p_a, RH_a). \quad (0.13)$$

By replacing the  $k$  constant in equation (0.7) with equation (0.13), Dalla Barba et al. [2] derived a revised  $D^2$ -law. It is worth noting that this revised model does not use any free fit parameter. The major difference between the classical and revised law relies on the assumptions made on droplet temperature. In the classical  $D^2$ -law this is assumed equal to the initial one. In the revised model, it results from the balance between the heat flux and latent enthalpy during the evaporation process. Considering an evaporating droplet with an initial temperature higher than, or equal to, the ambient temperature in quiescent air conditions, its temperature will tend to an asymptotic value, which is lower than the environmental temperature, after a short transition time. Hence, in the revised  $D^2$ -law, the droplet temperature is fixed and equal to this asymptotic value, instead of the initial one, that results in a constant evaporation rate lower than the one predicted by the classical model. The performance of this revised  $D^2$ -law has been tested against DNSs of turbulent water sprays with different dilute levels, as well as reference data of respiratory droplets from third parts, i.e. Ng et al. [9], exhibiting an excellent agreement. To further assess the reliability of the revised  $D^2$ -law in predicting the evaporation of a droplet we provide a comparison of our model against independent experimental data [8]. The experiments have been realized using an acoustic levitator under well-defined ambient and initial conditions, considering single water



**Figure 3.** Distance travelled by the front of a turbulent jet/puff reproduced by experimental data from [11]. The two stages that characterize the flow, jet (early stage) and puff (late stage), are visible. The scaling laws for the jet,  $L \propto t^{1/2}$ , and puff phase,  $L \propto t^{1/4}$ , are reported as references with black dashed lines. Qualitative visualizations obtained from experiments showing the instantaneous tracers concentration (black-high; white-low) at different times ( $t = 0.25$  s and  $t = 1.00$  s, respectively) are reported as representative of the jet/puff evolution.

and saliva droplet [8, 10]. In figure 2 the decay of the square droplet diameter of saliva droplets predicted by the classical model, the present one and the experimental results from Lieber et al. [8] are shown. Two different environmental conditions are considered showing an approximately linear decay. For both the cases, the revised  $D^2$ -law model shows superior performance than the classical one and very good agreement with the experimental data. As reported in Lieber et al. [8], a terminal size of around 25% of the droplet initial diameter, is reached at the end of the evaporation due to the non-volatile components inside the saliva droplet, like salts and protein. We attribute this reason to explain the slight deviation of the revised model from the experimental data at the late stage of evaporation. However, as mentioned in Dalla Barba et al. [2], some restrictions should be considered when using the revised  $D^2$ -law, i.e. single component droplets, micro/millimetre size, dilute regimes, and the different properties of turbulent jet/puff carrying the droplets and the ambient air. In fact, as shown in Figure 2B of the manuscript, the revised  $D^2$ -law fails to capture the mean behavior of droplet evaporation in low temperature and high relative humidity ambient conditions, which are strongly different from the initial jet ones. However, the obtained prediction is still much more accurate than the classical one, especially for long times.

Let consider equation (0.1) applied along the horizontal direction. If the droplet is sufficiently small, the term  $\tau_d$  approaches zero and equation (0.1) becomes  $u_d \simeq \bar{u}$ . Hence, we assume that, along the horizontal direction, droplets move with the same velocity of the carrier flow. To estimate the axial speed of the carrier flow, we split the evolution of the exhaled flow into two different stages, as can be seen in the Fig 3. From  $t = 0$  up to the time the flow is emitted from the oral cavity,  $t = t_{inj}$  (injection time), we model the flow as an axial, steady round jet for which a well-established, self-similar velocity profile is known [12]. On the other hand, for  $t > t_{inj}$ , we model the flow as a free turbulent puff. For the latter, the distance travelled by a Lagrangian tracer is known to scale with a power law of  $t^{1/4}$ ,  $L/L_0 \sim (t/t_0)^{1/4}$  [13]. In this frame, for  $t \leq t_{inj}$ , by neglecting possible two-way coupling effects, an estimate of the length covered by droplets carried by the jet can be obtained by considering the self-similar behaviour of the mean jet centerline velocity,  $U_c \simeq \bar{u}$ , and supposing that the droplet mean axial velocity is approximated

by  $u_d \simeq U_c$ :

$$\frac{U_c}{U_0} = \frac{2B}{\frac{x}{R_0} - \frac{x_0}{R_0}} \implies \frac{R_0}{U_0} \frac{d}{dt} \left( \frac{x_d}{R_0} \right) = \frac{2B}{\frac{x_d}{R_0} - \frac{x_0}{R_0}}, \quad (0.14)$$

with  $B \simeq 6$  a universal constant,  $x_0$  the so-called jet virtual origin [14],  $x_d$  the droplet position along the jet axis,  $U_0$  the bulk velocity at the exit of the oral cavity and  $R_0$  the mouth radius (under the assumption of a nearly circular orifice). Then, integrating equation (0.14) and assuming a vanishing virtual origin,  $x_0/R_0 \simeq 0$ , it leads to:

$$L_d = x_d = \sqrt{4BU_0R_0} t^{\frac{1}{2}}. \quad (0.15)$$

For  $t > t_{inj}$ , we suppose that the exhaled moist air behaves like a puff. For the latter, the distance travelled by a Lagrangian tracer scales as  $L/L_0 \sim (t/t_0)^{1/4}$  and its initial value has to match the one obtained by equation (0.15). Hence,

$$L_d = x_d = \sqrt{4BU_0R_0} t_{inj}^{\frac{1}{4}} t^{\frac{1}{4}}. \quad (0.16)$$

Finally, let consider equation (0.1) along the vertical direction. We suppose that large evaporating droplets, acting as ballistic particles, reach their terminal settling velocity with a negligible transient time. Hence, by setting  $du_d/dt \simeq 0$  and  $\bar{u} = 0$ , considering the definition of the droplet relaxation time,  $\tau_d = \rho_d D_d^2 / (18\bar{\mu})$ , as well as equation (0.7) and (0.13), we obtain:

$$u_d(t) = \frac{1}{18} \frac{f}{\bar{\mu}} (\rho_d - \bar{\rho}) g D_d^2, \quad f = \frac{1}{1 + 0.15 Re_d^{0.687}}. \quad (0.17)$$

By setting a null initial vertical velocity, the falling distance displaced by droplets,  $H_d(t)$ , can be obtained by integrating equation (0.17):

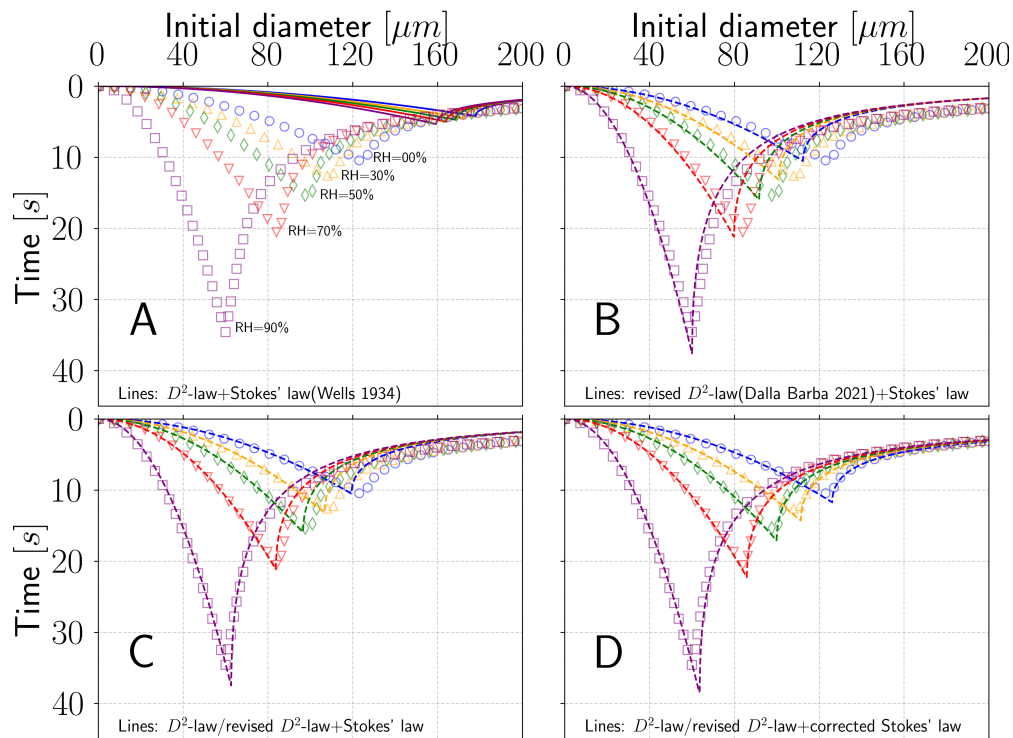
$$H_d(t) = \frac{f}{18} \frac{\rho_d - \bar{\rho}}{\bar{\mu}} g (D_{d,0}^2 t - \frac{k}{2} t^2) \quad (0.18)$$

Finally, the latter can be solved for the settling time,  $t_s$ , when the vertical distance is specified, e.g.  $H_d = 2m$ . The solution is provided in the following, skipping algebraic manipulation:

$$t_s = \frac{1}{k} \left( D_{d,0}^2 - \sqrt{D_{d,0}^4 - \frac{36\bar{\mu}kH_d}{(\rho_d - \bar{\rho})gf}} \right). \quad (0.19)$$

## Model description

To further explain how the present model was developed step by step based on the classical framework, we show in figure 4 a comparison of the lifetime of free-falling, evaporating water droplets estimated with different models (lines), from A) to D), against the benchmarking data (symbols) collected from Xie's results [15]. The seminal theory introduced by Wells in the 1930s, based on the classical  $D^2$ -law and Stokes' law, highly overestimates droplet evaporation rate, leading to the prediction of very short evaporation times, as reported by recent studies [7, 11, 16, 17] and highlighted in Panel A of figure 4. Simply replacing the classical  $D^2$ -law with the revised one [2], a relevant improvement is observed, see Panel B. However, some discrepancies still subsist; these are attributed to the non-negligible transition time for droplets to reach the asymptotic temperature and the inaccuracy of Stokes' law in describing the settling velocity of evaporating droplets with inertia. These two deficiencies have been mitigated by considering a two-stage evaporation model and a fixed drag correction factor, as showed in Panel C and D of figure 4, sequentially.



**Figure 4.** Comparisons of the lifetime of free-falling, evaporating water droplets with different initial sizes under different environmental conditions: A) Wells Theory; B) Revised  $D^2$ -law coupled with Stokes' law; C) Two-stages  $D^2$ -law coupled with Stokes' law; D) Two-stages  $D^2$ -law coupled with corrected Stokes' law. These predictions are shown in lines, whereas the symbols represent benchmarking data collected from Xie's results [15]. It is worth remarking that the prediction accuracy of the classical model can be improved by taking into account the revised  $D^2$ -law, the two-stages evaporation model and a fixed drag correction factor  $f$ .

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