Criterion of drop fragmentation at a collision with a solid target (numerical simulation and experiment)

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Abstract. This paper is devoted to the study of the deformation and fragmentation of liquid droplets when they collide with masks and filters used for protection against infected droplets. In this paper, the local collision of a drop with a mask or filter is modeled numerically and experimentally by the example of the drop impact on a small obstacle. Studies allow tracing the fragmentation of oral and bronchial fluids and their transformation into the number of tiny droplets that spread infection in the air.

1. Introduction
Breathing, coughing, and sneezing cause the release of droplets of saliva and bronchial mucus, which can fragment. Many viruses, including COVID-19, (whose size is about 100–120 nm) live only in a liquid environment. The minimum size of droplets with virus carriers is comparable to the size of the pores of masks (about 0.1–10 microns), so it is important to study the hydrodynamics and fragmentation of droplets when passing through protective masks, filters and clothing. This article is devoted to the study of the deformation and fragmentation of liquid droplets when they collide with masks and filters that protect against the ingress of infected airborne droplets. In this paper, the local collision of a drop with a mask or filter is modeled numerically and experimentally by the example of the drop impact on a small obstacle. Studies allow tracing the fragmentation of oral and bronchial fluids and their transformation into the number of tiny droplets that spread infection in the air. In reality, the infected droplets falling on masks and filters have approximately the same values of the Weber number.

2. Problem statement and mathematical model
The nature of the spreading of the drop is determined by the ratio and interaction of the forces of inertia, viscosity and surface tension, as well as the wetting angle of the surface (in the calculations, the wetting angle was equal to 90°).

The problem is characterized by dimensionless Reynolds \( Re = \frac{\rho \nu_i d_i}{\mu} \) and Weber \( We = \frac{\rho 
u_i^2 d_i}{\sigma} \) numbers, where \( \rho \) is the density, \( \nu_i \) is the drop rate of incidence, \( d_i \) is the drop diameter, \( \mu \) is the viscosity, and \( \sigma \) is the surface tension coefficient. For water droplets, the properties are set as follows: \( \rho = 1000 \text{ kg/m}^3 \) - density, \( \mu = 10^{-3} \text{ kg/m sec} \), and \( \sigma = 0.072 \text{ N/m} \).

A scheme of the drop motion model is shown in Figure 1a. Fig. 1b shows the experimental data (on the left) and the results of 3D modeling (on the right) of the water drop spreading (\( \nu_i = 3.87 \text{ m/s}, d_i = 2.67 \text{ mm}, d_t = 4 \text{ mm} \)), demonstrating of the formation of a lamella with a rim jet and secondary
drops at time moment $t = 1$ ms. For oral and bronchial water-based drops of typical diameter $d_i = 100\mu m$ and impact velocity $v_i = 10$ m/s, the Weber number of the impact $We_i = \rho v_i^2 d_i / \sigma = 139$. Therefore, the collision is controlled by inertia and capillarity, while the influence of all other factors is negligible.

![Image](https://via.placeholder.com/150)

**Figure 1.** a) Liquid lamella formed upon a liquid drop impact on a small disc-like target, b) spreading of a water drop ($v_i = 3.87$ m/s, $d_i = 1$ mm) (experiment is on the left, and 3D modeling is on the right (velocity module isolines are shown)).

The mathematical model is based on solving the system of 3D and two-dimensional Navier-Stokes equations in the axisymmetric approximation. For 2D case for a two-phase gas-liquid system in the approximation of the “mixture” model [1] Navier-Stokes equations may be written in the form:

\[
\frac{\partial u_1}{\partial t} + \frac{\partial u_1}{\partial x_1} + \frac{\partial u_1}{\partial x_2} = 0
\]

\[
\frac{d(\rho u_1)}{dt} = -\frac{\partial p}{\partial x_1} + \frac{1}{x_1 \partial x_1} \left( x_1 \mu \frac{\partial u_1}{\partial x_1} + \frac{\partial}{\partial x_2} \left( \frac{\partial u_2}{\partial x_2} - \frac{\partial u_1}{x_1^2} \right) \right) - \frac{\partial u_1}{x_1^2} + F_1
\]

\[
\frac{d(\rho u_2)}{dt} = -\frac{\partial p}{\partial x_2} + \frac{1}{x_1 \partial x_1} \left( x_1 \mu \frac{\partial u_2}{\partial x_2} + \frac{\partial}{\partial x_2} \left( \frac{\partial u_1}{\partial x_2} \right) \right) + F_2
\]

where $df / dt = (\partial f / \partial t + v_i \partial f / \partial r + v_z \partial f / \partial z)$ is the substantial derivative, $x_1 \equiv r$, $x_2 \equiv z$ are the radial and axial coordinates, $u_1 \equiv v_r$, $u_2 \equiv v_z$ are the velocity vector components $u(u_1, u_2)$, $t$ is the time, $p$ is the pressure, $\rho$ is the density, $\mu$ is the dynamic viscosity coefficient, and $F_1, F_2$ are the radial and axial components of external force $F(F_1, F_2)$, operating in a narrow zone along the gas-liquid interface.

To describe the two-phase gas-liquid system, we used the system of equations (1-3) with one equation for momentum transfer under the assumption of a “mixture” model [1] with averaged velocities $u = \varepsilon u_{gas} + (1-\varepsilon) u_{liquid}$, density $\rho = \varepsilon \rho_{gas} + (1-\varepsilon) \rho_{liquid}$, and viscosity $\mu = \varepsilon \mu_{gas} + (1-\varepsilon) \mu_{liquid}$, where the values with the index ‘gas’ refer to gas, and with the index ‘liquid’ refer to liquid. The volume fraction of liquid $\varepsilon (0 < \varepsilon < 1)$ was determined from the solution of the transfer equation: $\partial \varepsilon / \partial t + u_i \partial \varepsilon / \partial x_i + u_z \partial \varepsilon / \partial x_2 = 0$.

The boundary conditions at the gas–liquid interface were determined from the equilibrium condition of surface forces and pressure [1]:

\[(p_1 - p_2 + \sigma \kappa)n_j = (\tau_{ij} - \tau_{2j})n_j\]
where $\sigma$ is the surface tension coefficient assumed to be constant, $p_1$, $p_2$ are the fluid and gas pressures, $\kappa = 1/R_1 + 1/R_2$ is the surface curvature where $R_1$, $R_2$ are the radii of curvature for liquid and gas, $\mathbf{n}$ is the unit normal vector directed into the second fluid, $\tau_{\omega\phi}$ is the viscous stress tensor, and index $\alpha$ denotes: $\alpha=1$ – liquid, $\alpha=2$ – air. Condition (4) is written for a constant coefficient $\sigma$.

The conditions for the absence of friction are set at external boundaries of the computational domain, the condition of symmetry on the axis, and condition (4) at the interface of the two-phase liquid-air system. The modeling of the change in the shape of the gas-liquid interface was performed using the model of liquid volumes (VOF - Volume Of Fluid method). The interface was determined by the VOF method with increased resolution and taking into account surface forces by the CSF method (Continuum Surface Force) [2]. The CSF method allows removing the singularity in the case of turning the radius of curvature of the interface surface to zero and increasing the accuracy of the calculations [2]. When solving the problem, condition (4) at the interphase boundary was taken into account through an additional local bulk force $\mathbf{F}$ on the right side of the momentum transfer equation (2) - (3). The force $\mathbf{F}$ acts only in a very narrow area, enclosed along an interface line of width $\Delta h$. At every point $l_i$ of interface lines $l$, at $\Delta h$ striving to zero, the force $\mathbf{F}$ can be written as $\mathbf{F}(l_i) = \sigma \kappa(l_i) \mathbf{n}(l_i)$, where $\kappa(l_i)$ is the interface curvature at a point $l_i$, and $\mathbf{n}(l_i)$ is the normal to the site at the interface point $l_i$ [2]. For the numerical solution of the Navier-Stokes equations, a program code was used applying the control volume method [3]. Verification of the program code for two-phase flows was carried out on several test tasks, in particular, some of which were indicated in papers [4, 6].

3. Results

In numerical simulations and in laboratory experiments, the similarity was provided by water droplets with a diameter of 2.8 mm and impact velocities of 1.88-3.57 m/s, which correspond to the Weber numbers $We_i = 137 - 267$. As a result of the collision, a round liquid lamella is formed with a torus-shaped roller on the edge (the edge jet) (Fig. 1–3). The lamella first expands, and then tighten back to the target, forming radially directed liquid “fingers” on the edge jet. At low impact speeds, the “fingers” retain continuity, while at a sufficiently high speed, the “fingers” fragment into secondary drops [4-7]. The formation of secondary droplets (splashing) occurs both when the lamella expands and when it tightens back, and the secondary droplets can move in opposite directions. Fig. 2 and Fig. 3 show the numerical and experimental results of the impact of a drop on a target for various Weber numbers. Experiments have shown [7], and numerical simulations have confirmed that the critical Weber number corresponding to the transition to lamella spattering lies in the range (137, 206).

The results of studies have shown that the infection may spread due to the disintegration of droplets when hitting solid obstacles in real natural conditions (in-situ). Drops of biological fluids collide with the material of masks and filters with approximately the same Weber numbers $We_i \approx 100$. Thus, the studied processes of droplet fragmentation in the experiments (laboratory and numerical), and occurring in reality, have the same mechanisms. The transition to splashing a drop of liquid onto secondary drops occurs at the Weber numbers $We_i > We_i^*$, where $We_i^* \subset (137, 206)$.

These studies indicate the existence of a critical Weber number $We_i^*$, which, if exceeding $We_i > We_i^*$, will cause fragmentation of the oral and bronchial fluids and their transformation into a large number of tiny droplets that spread the infection in the air.
Figure 2. Patterns of droplet spreading after an impact on solid target \((d_i=2.8\ \text{mm}, \ \nu_i=1.88\ \text{m/s}, \ \text{We}_i=137)\) for different time moments (on the left – calculation, on the right – experiment [7]).

Figure 3. Patterns of droplet spreading after an impact on solid target \((d_i=2.8\ \text{mm}, \ \nu_i=2.3\ \text{m/s}, \ \text{We}_i=206)\) for different time moments (on the left – calculation, on the right – experiment [7]).

Conclusions

The transition to liquid drop splashing onto secondary drops occurs at the Weber numbers \(\text{We}_i > \text{We}^*_i\), where \(\text{We}^*_i \subset (137, 206)\). These studies indicate the existence of a critical Weber number \(\text{We}^*_i\), which, if exceeding \(\text{We}_i > \text{We}^*_i\), will cause fragmentation of the oral and bronchial fluids and their transformation into a large number of tiny droplets that spread the infection in the air. The results obtained can be used to calculate social distance in various life situations.

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