DNS of ethanol droplet impact onto a smooth surface

Rishav Saha*, Cemre Inal, Bernhard Weigand
Institute of Aerospace Thermodynamics, University of Stuttgart, Germany
*Corresponding author: rishav.saha@itlr.uni-stuttgart.de

Abstract

In this work, we studied the ethanol droplet spreading process and its dependence on the droplet Weber and Reynolds numbers. We investigated the spreading factor β [1], a critical parameter for characterizing droplet dynamics upon impact, for ethanol droplets over a Weber number range from 35 to 315, using Direct Numerical Simulation (DNS). Subsequently, the DNS results are validated against established empirical correlations. The spreading factor is then studied and compared for ethanol and water droplets. The study employs a Computational Fluid Dynamics (CFD) framework to simulate the impact process, solving the incompressible Navier-Stokes equations using the Finite-Volume method. The gas–liquid interface is defined using the Volume-of-Fluid (VOF) method [2], and the Piecewise Linear Interface Calculation (PLIC) method [3] is employed for interface reconstruction. The DNS tool Free Surface 3D [4] (FS3D), an in-house code at the Institute of Aerospace Thermodynamics, University of Stuttgart, is utilized.

Introduction

When a droplet impacts a surface with a high impact velocity, the droplet mostly splashes and forms secondary droplets, and some portion of the liquid sticks on the surface [1]. Whereas a droplet with a relatively lower impact velocity spreads on the surface without splashing. In this work, we investigated droplets with relatively lower impact velocity within the spreading regime. During this spreading process, the key dimensionless parameters [1] influencing the dynamics, the Weber number (We) and the Reynolds number (Re) are defined as follows:

$$We = (\rho D_0 U_0^2) / \sigma \quad , \qquad (1)$$

$$Re = (\rho D_0 U_0) / \mu \quad , \qquad (2)$$

where ρ is the liquid density, U_0 is the droplet impact velocity, D_0 is the initial droplet diameter, σ is the interface tension, and μ is the dynamic viscosity of the liquid. Figure 1 shows a schematic of a droplet impacting a smooth surface.

One of the most important dimensionless quantities for studying the impact process is the spreading factor [1]. The spreading factor β quantifies the extent to which a droplet spreads upon impact and is defined as the ratio of the maximum spreading diameter D_{max} to the initial droplet diameter D_0:

$$\beta = D_{max} / D_0 \quad . \qquad (3)$$

The spreading factor is influenced by both the Weber and Reynolds numbers. A higher value of the Weber and Reynolds numbers generally leads to an increased β. In many previous studies on the determination of the spreading factor β, various empirical formulas have been proposed for a range of Weber and Reynolds numbers, derived from experiments and analytical methods [5, 6, 7]. Table 1 summarizes the applicable ranges of Weber and Reynolds numbers for the empirical correlations from previous studies [5, 6, 7].

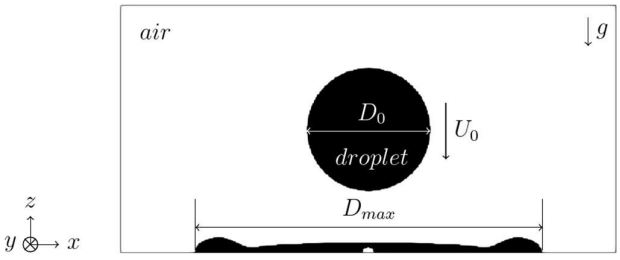

Figure 1. Schematic diagram of a droplet impacting onto a smooth surface. D_0 is the initial droplet diameter, impacting with a velocity of U_0, and D_{max} is the maximum spreading diameter. The liquid is shown in black.

Correlations		We valid range	Re valid range
$\beta = 1.27\ (Re^2\ Oh)^{0.122}$	Seo et al. [5]	12 < We < 1457	560 < Re < 6115
$\beta = 0.55\ (Re\ We^{0.5})^{0.18}$	Tian and Chen [6]	1.5 < We < 673	196 < Re <4104
$\beta = (Re^{0.2}\ We^{0.5}) / (7.6 + We^{0.5})$	Lee et al. [7]	1 < We < 1300	450 < Re < 18000

Table 1. Correlations are provided along with the corresponding ranges of Weber and Reynolds numbers for which the respective correlations of the spreading factor (β) are valid. The Ohnesorge number is defined as $Oh = We^{0.5} / Re$.

In this study, DNS were conducted for an ethanol droplet of D_0 = 1 mm impacting at different impact velocities onto a smooth surface, with a Weber number range of 35 to 315 (see Table 2) to study the spreading factor β. The flow is assumed to be incompressible and Newtonian, with no phase change. These results were validated using empirical correlations and compared with simulation results for water droplets. All simulations were performed for a flat surface with a static contact angle of 90°. Simulatons were run on the HPE Apollo Hawk supercomputer at the High-Performance Computing Center Stuttgart (HLRS), with a total simulation time of 3 ms for each case.

Results and Outlook

Table 2 presents the five simulated cases for ethanol droplets along with the corresponding DNS results. Figure 2 shows the validation of the DNS results for the spreading factor β, against empirical correlations [5,6,7]. A comparison of the spreading factors between ethanol and water droplet is also included in the same figure.

Case	I	II	III	IV	V
We	35	79	141	220	315
$Re^{0.2}$	3.66	3.97	4.2	4.39	4.56
β	2.45	2.85	3.18	3.45	3.69
$\tau_\beta = t\ (U_0 / D_0)$	1.55	2	2.35	2.75	3.05

Table 2. Summary of simulation parameters and corresponding results for ethanol droplet impact onto a smooth surface. The table lists the Weber number, Reynolds number to the power of 0.2, spreading factor β, and the dimensionless maximum spreading time τ_β for all five cases. Here, t is the physical time.

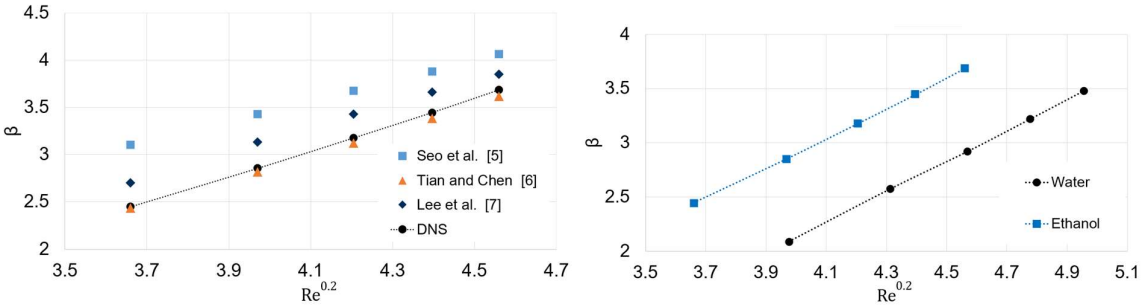

Figure 2. Left: Validation of the spreading factor (β) obtained from DNS for various Weber and Reynolds numbers, compared with different empirical models for ethanol droplets. Right: Comparison of the spreading factor predicted using DNS for ethanol and water droplet impacts.

It is observed that the spreading factor increases with rising Weber and Reynolds numbers within the viscous flow regime [1]. In addition, different liquid droplet experiences different spreading factor upon similar impact conditions. Therefore, to understanding the interplay between viscous, inertial and capillary forces during this dynamic process, different liquids must be studied. In future, FC-72 (refrigerant perfluorohexane) droplet impact onto a hydrophilic surface is simulated using dynamic contact angle models to predict β and dynamic spreading using DNS.

References

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