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Tachyothesis Theory and Molecular Dynamics Simulation of Shock-Induced Catastrophic Droplet Vaporization

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Spray detonation involves strong shock waves impacting fuel droplets, which undergo vaporization, mixing, and subsequent exothermic reaction. Modeling spray detonation requires understanding the mechanism and timescales involved in shock-induced droplet vaporization. Droplet breakup in detonation relevant conditions, which involves shocks of M~5, is in the 'catastrophic' or high Weber (We) number regime where surface tension effects play a minor role. Experiments [1] and molecular dynamics (MD) simulations [2] have demonstrated that the vaporization mechanism of shock-impacted droplets is similar across a wide range of droplet diameters, from nm to mm. MD simulations of *n*-dodecane droplets 5-25 nm in diameter impacted by an M=5 N_2 shock, where surface tension and We number effects are both more pronounced than larger droplets, show rapid flattening of the droplet and acceleration and expansion, in agreement with experimental observations made for much larger droplets impacted by similar shocks. The droplets exhibit non-equilibrium and supercritical behaviors: *n*-dodecane molecules are translationally hot and vibrationally cold upon shock impact, and they appear in molecular clusters at a somewhat later stage of the shock impact. The acceleration and heating of the droplet occur due to post-shock gas impingement and compression, which transfers mechanical work to the droplet, leading to spatial displacement and thermal energy injection and subsequent vaporization at a rate substantially faster than what would be predicted by Stokes' drag and the d^2-law of evaporation, respectively.

Based on the above understanding, an analytical, physics-based *tachyothesis* theory was developed to describe coupled momentum and energy transfer to shock-impacted liquid droplets. Considering full momentum and energy accommodation from the post-shock flow enables *a priori* predictions of droplet displacement and vaporization. A skin friction correction, fit to weak shock experiments by Ranger and Nicholls [1], is included to extend the applicability of the theory to shocks of strength down to M=1.5. The droplet vaporization time is found to depend on a shape response parameter, which describes the rate of droplet flattening and hence energy injection. The shape response parameter can be measured experimentally and primarily depends on the pre-shock thermodynamic state. Therefore, it is possible to carry out canonical experiments to obtain the value of this parameter and in doing so, enable *a priori* predictions for droplet drag and vaporization for liquid droplets from both MD simulations of 5-25 nm sized *n*-dodecane droplets and experiments over a wide range of shock strength, pre-shock pressure, and droplet materials, The *tachyothesis* theory has been implemented in continuum simulations of two-phase detonation, as demonstrated recently [3].

[1] Ranger AA and Nicholls JA. Aerodynamic shattering of liquid drops. AIAA Journal. 1969;7.2:285-290.
[2] Kateris N et al. Shock-initiated fragmentation of *n*-dodecane nano-droplets: a molecular dynamics study. 29th ICDERS. 2023;268.
[3] Dammati SS et al. Numerical simulations of non-ideal spray detonations in jet fuels with a shock-droplet interaction model. AIAA SCITECH 2025 Forum. 2025;0388.