

INTERACTIONS OF LIQUID DROPS
WITH GAS FLOW — REVIEW

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Introduction

Breakup of drops and jets is recognized to be one of the major factors contributing to combustion of liquid fuels in flows, particularly in high-speed flows inherent in rocket engines and detonation waves. Reduction of the drop size and increase in the specific surface of evaporating drops, that may be of the same order of magnitude, highly intensifies mass transfer. The number of publications in which the problem has been tackled both theoretically and experimentally counts more than one hundred, including a few comprehensive reviews. Therefore in the present work, emphasis is made on analyzing those of them that are directly relevant to pulse detonation engines, among them enhancement of fuel–air mixing on the molecular level prior to ignition and in the reaction zone of detonation waves spreading in sprays. The breakup modes controlling mass transfer in these two zones of the combustion chamber appreciably differ, therefore they should be considered separately. Also, other interactions between liquid drops and gas flow, that is, vaporization, ignition, and combustion are discussed.

Breakup

As follows from physical reasoning and dimensional analysis, breakup is governed by the following basic dimensionless numbers representing ratios of the forces: aerodynamic force to surface tension or Weber number $We = \rho V^2 D / \sigma$, aerodynamic force to viscous force in the gas phase or Reynolds number $Re = VD\rho/\mu$, and viscous force to surface tension in the liquid phase or Ohnesorge number $Oh = \mu_l / (\rho_l D \sigma)^{1/2}$, where D is the initial drop diameter, μ_l is viscosity of the liquid phase, σ is the surface tension, ρ_l is the liquid density, and V , μ , and ρ are the free stream gas velocity (with respect to the drop), viscosity, and density, respectively. Ohnesorge number comes into play when viscosity of liquid is high therefore, when breakup of such inviscid liquids as hydrocarbons for which $Oh < 0.1$ are considered, its effect on mass transfer can be neglected. Generally, depending on the Weber number, the breakup modes look as shown in Fig. 1.

The figure illustrates schematically the sequence of breakup stages representing only their major features, many details remaining beyond the picture. Although the conditions for critical Weber numbers and for each particular breakup mode reported in various publications differ, the discrepancy is not significant to deserve special discussion. As far as detonation waves spreading in sprays are concerned, the main droplet breakup mode is combination of stripping and Rayleigh–Taylor instability modes (Fig. 1c). These modes produce two sorts of secondary drops: micromist, as a result of disintegration of the stripped sheet, and larger drops arising after perforation of the parent drop with gaseous “fingers” due to Rayleigh–Taylor instability and disintegration of the perforated disc.

As follows from linear analysis, there is a minimum wave length of instability waves $\lambda = 2\pi(\sigma/\rho_{liq}a)^{1/2}$ (where a is the droplet acceleration) below which their amplitude does not grow [2], hence droplets of size less than λ are not subjected to Rayleigh–Taylor instability. According to [2], behind a shock wave with Mach number $M = 3$, λ ranges between 23 and 63 μm . Unfortunately, available experimental data pertain to larger drops, therefore breakup patterns of fine drops call for additional experimental verification.

Breakup modes inherent in lower We numbers are important at the stage of mixture preparation, e.g., when injecting fuel in an air stream,

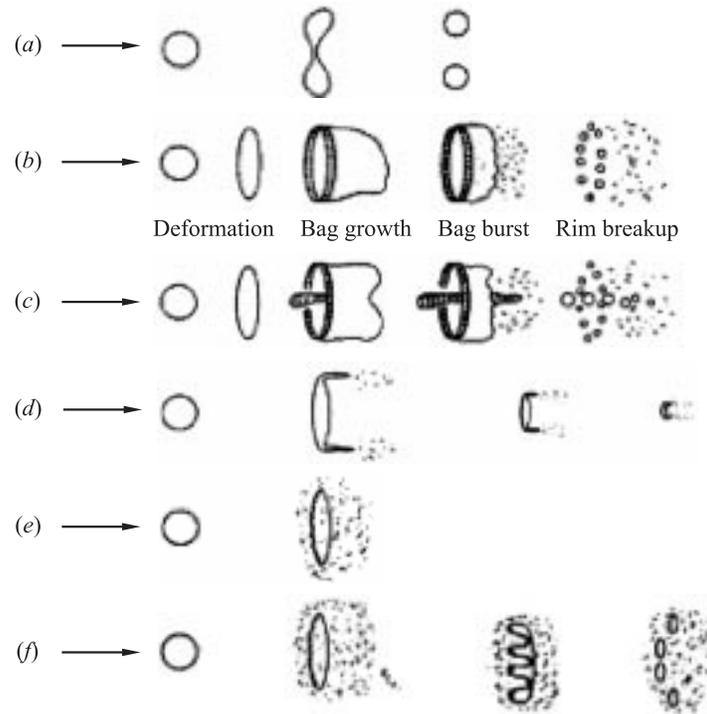


Figure 1 Mechanisms of breakup of low-viscosity liquid drops observed experimentally [1]: (a) vibrational breakup $We < 12$, (b) bag breakup $12 < We < 50$, (c) bag-and-stamen breakup $50 < We < 100$, (d) sheet stripping $100 < We < 350$, (e) wave crest stripping $350 < We < 2670$, and (f) catastrophic breakup $We > 2670$. Arrow shows the flow direction

but usually they do not result in such a dramatic increase of the evaporating surface area as do the stripping and Raileigh–Taylor instability modes. But there is one process where these modes can significantly change the burning process. This is transition from deflagration of a spray to detonation, which is greatly stimulated by sending weak shock waves in a burning spray.

Mixing

The most important question to be answered for detonations is how fast the fuel is mixed with oxidizer on molecular level, because diffusion burning of drops of size exceeding $10\ \mu\text{m}$ takes too long time to provide the needed rate of energy supply to the shock leading to detonation. The answer to this question presumes knowledge of (i) the total breakup times and (ii) state and geometry of the two-phase cloud arising after the breakup. The representative time of drop deformation, and hence of breakup, following from dimensional analysis is $t^* = V(\rho_{\text{liq}}/\rho_{\text{gas}})^{1/2}/D$, therefore for convenience, the total breakup time is usually expressed in t^* units. The reduced breakup times τ for low-viscosity liquids range between 3.5 and 6. The authors of [1] report empirical formulae relating τ to the We number:

$$\begin{aligned}\tau &= 6(\text{We} - 12)^{-0.25} && \text{at } 12 \leq \text{We} \leq 18 \\ \tau &= 2.45(\text{We} - 12)^{0.25} && \text{at } 18 \leq \text{We} \leq 45 \\ \tau &= 14.1(\text{We} - 12)^{-0.25} && \text{at } 45 \leq \text{We} \leq 351 \\ \tau &= 0.766(\text{We} - 12)^{0.25} && \text{at } 351 \leq \text{We} \leq 2670 \\ \tau &= 5.5 && \text{at } \text{We} \geq 2670\end{aligned}$$

Thus, the fluid in the wake of a broken up drop is a mixture of the free-stream gas, fuel vapor, and secondary droplets of various size. Photographic studies fail to provide information about the state of the material in the drop wake because of strong light scattering by dispersed material, even X-ray diagnostics [3] furnishes data on the overall density of the mixture saying nothing about the structure and aggregate state of the mixture.

Vaporization

Figure 2 shows a photograph of a shattered drop in the shock-induced air flow. The totally opaque wake of the drop consists of very fine droplets. The amount of air entrained in the wake at $\tau = 3.1$ is estimated at about 450 volumes of the original drop. If it were hydrocarbon drop, rather than water, the equivalence ratio Φ averaged over the wake would be about 5.

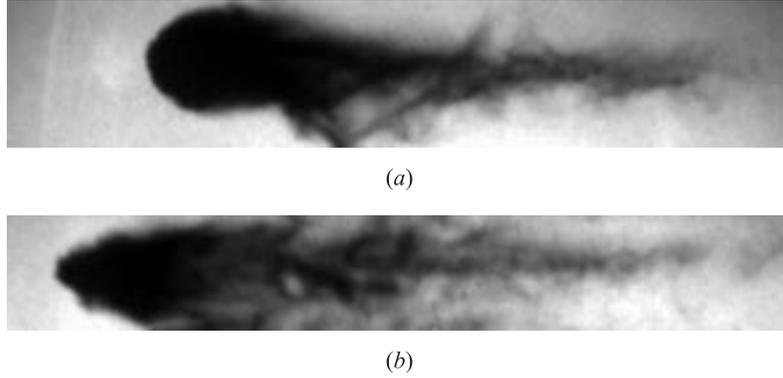


Figure 2 Water drop (0.3 mm in diameter) shattered behind a Mach 2.4 shock wave at 22 μs (*a*) and 27 μs (*b*), $\tau = 2.5$ and 3.1, respectively

Analysis of drop vaporization in such dense drop suspensions indicates [4] that drop lifetime increases considerably as compared to the isolated drop in an unconfined atmosphere. For example, Fig. 3 shows the calculated time histories of the squared drop diameter depending on Φ . Three important findings are worth mentioning: in the spray, (*i*) drops evaporate slower, (*ii*) the deviations from the classical d^2 -law increase as Φ increases, and (*iii*) at certain Φ , drops evaporate only partly.

The latter finding is due to a considerable screening effect of neighboring drops in the cloud resulting in vapor saturation conditions in the interdrop space. Slower vaporization of individual drops has been observed in experiments with linear drop arrays [5]. It is natural to anticipate that similar effects are inherent in the micromist behind a shattered parent drop. Moreover, one can suspect that drops are mostly concentrated at the wake periphery. Unfortunately, this stage of the process is not properly studied yet to propose reliable relationships for calculating its rate.

Apart from the traditional combination of micromist and larger fragments arising as a result of stripping and Rayleigh–Taylor instability mechanisms, the authors of [6] propose a flash vaporization mechanism caused by low pressure and high temperature at the leeside of

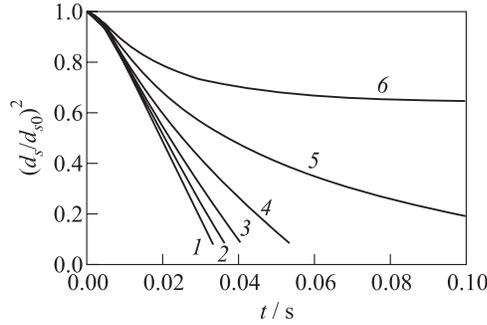


Figure 3 Predicted time histories of normalized surface of an *n*-heptane drop evaporating in air as a function of the equivalence ratio Φ [4]. Initial parameters: drop diameter $d_{s0} = 70 \mu\text{m}$, drop temperature $T_{l0} = 293.15 \text{ K}$, gas temperature $T_{g0} = 573.15 \text{ K}$, and pressure $p = 0.1 \text{ MPa}$. 1 — $\Phi = 0$ (isolated drop), 2 — 1.06, 3 — 2.12, 4 — 4.25, 5 — 8.5, and 6 — $\Phi = 17.0$

liquid drops in supersonic flows. The sources of this phenomenon are: (i) rarefaction of the gas as it passes over the drop, (ii) fast drop acceleration, (iii) high tension in the drop produced by extensional motions of matter stripped from it, (iv) frictional heating which is inevitable for huge strains in the drop, and (v) heating of thin sheets torn from the drop periphery by hot gas. Flash evaporation arises at early breakup stage and rapidly relaxes, so that vapor can recondense producing again micromist.

Ignition

Of great importance for the detonation process is that, whatever the prevailing mechanism of liquid atomization, the major heat supporting the wave is released in the boundary layer surrounding the drop wake which, according to experimental observations, is nearly of a conical shape. Thus both numerical simulations and evidence derived from shock tube experiments suggest three major stages of heat release in detonation waves spreading in sprays: (i) drop breakup, (ii) ignition of the mixture at the wake periphery, and (iii) diffusion-controlled fuel burning in the wake.

Which of the stages is rate controlling can be assessed from simple considerations. Breakup of drops 100 μm in diameter is completed within less than 10 μs behind the lead shock of a typical fuel-air detonation wave spreading at a velocity of 1600 m/s at atmospheric pressure, the total breakup time of smaller drops is even shorter. However, the pressure measured behind detonation waves in sprays of low-volatility fuels shows that the so-called von Neumann spike where the contribution of the reaction heat to flow characteristics is insignificant lasts no less than 100 μs . Hence, heat-release rate behind fuel-air detonation waves in sprays with practically attained drop sizes is controlled by the other two stages.

Mixture self-ignition is reasonably assumed to occur at the periphery of the cloud arising in the course of drop breakup because the gas in the wake is colder than the free-stream gas and fuel-oxidizer mixture capable of self-igniting exists only at the boundary between the free-stream and stripped droplet material. Rough estimates [7] show that the amount of fuel mixed with air in this boundary layer is small: no more than 16% over the total breakup time for 100-micrometer particles.

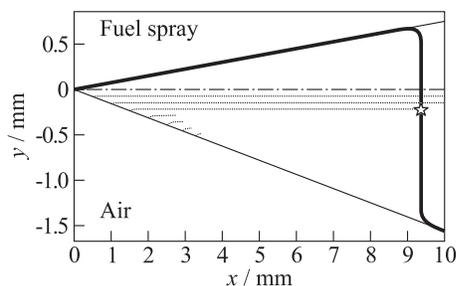


Figure 4 Predicted self-ignition location in the planar, isothermal, turbulent mixing layer of a fine fuel spray with air [8, 9]. Thin solid lines show the boundaries of the mixing layer. Thick solid curve denotes the locus of the limiting normalized preexplosion heating $\varepsilon = RT/E = 0.05$ (T is the temperature, E is the activation energy, and R is the gas constant). Dotted curves show the predicted mean trajectories of notional particles in the mixing layer. Star denotes the self-ignition location, where the notional particle residence time t is equal to ignition delay τ_i

Self-ignition in the boundary layer is controlled by chemical kinetics and may occur either after breakup or during it after an induction period, which can be approximately calculated using the free-stream temperature and pressure. For example, Fig. 4 shows the predicted self-ignition location (denoted by a star) in the planar, isothermal, turbulent mixing layer of a fine fuel spray in air [8, 9]. In the calculations, the following values of governing parameters were used: air density 30 kg/m^3 , fuel density 850 kg/m^3 , activation energy 8800 cal/mol , temperature 900 K , pressure 40 atm , and fuel spray velocity at the nozzle exit 100 m/s .

Ignition occurs at the periphery of the mixing layer at a distance of about 9 mm from the layer origin and 1.2 mm from the outer (air) boundary of the layer. Although the study in [8, 9] deals with the Diesel spray, the results obtained can be readily applicable to the self-ignition phenomenon in the cone-like mixing layer attached to shattered drops behind a detonation wave.

Combustion

Uncertainties in the ignition delay caused by nonisothermal conditions in the mixing layer cannot seriously affect the detonation wave parameters because self-ignition only starts the major energy release. After ignition, the cloud of very fine droplets in the wake of a parent drop (see Fig. 2) should burn in the diffusion controlled regime. In view of this, laminar droplet burning is one of the contributors to the overall heat release behind heterogeneous detonations because at the periphery of the mixing layer, droplets move at nearly the same velocity as does the gas.

As mentioned above, the mixture in the shattered drop wake is essentially fuel rich, which means that burning of fuel in the wake requires some oxygen to come from the free-stream. Similar to vaporization, combustion in dense drop suspensions is very sensitive to the drop loading ratio. The lifetime of burning drops also increases with Φ . Moreover, temperature in the interdrop space behaves very different from that typical for the isolated drop, other conditions being equal. For example, Fig. 5 shows the calculated time histories of the maximum temperature around burning drops depending on Φ [10].

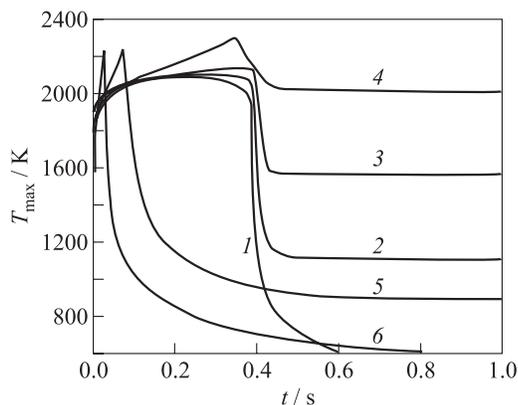


Figure 5 Predicted time histories of the maximum temperature around burning drops in suspension depending on Φ [10]. Initial parameters: $d_{s0} = 500 \mu\text{m}$, $T_{i0} = T_{g0} = 293.15 \text{ K}$, and $p = 0.1 \text{ MPa}$: 1 — $\Phi = 0$ (isolated drop), 2 — 0.32, 3 — 0.55, 4 — 1.1, 5 — 5.3, and 6 — $\Phi = 18.5$

The maximum temperature in drop suspension can be considerably higher than around an isolated drop. In the near-stoichiometric suspension (curve 4), the maximum temperature in the interdrop space remains constant at a level of about 2000 K, whereas for the isolated drop (curve 1), it falls down rapidly to the ambient temperature after drop burnout. In fuel-rich suspensions (curves 5 and 6), only a part of fuel is burned and the remaining fuel is vaporized and accumulated in the interdrop space together with combustion products. As the temperature in the interdrop space is high, fuel vapor can partly decompose to more reactive intermediate species. With thermal expansion and turbulent dispersion of the burning cloud, oxygen is engulfed into the cloud giving rise to high rates of gas-phase chemical conversion. Unfortunately, this mechanism of the heat-release process in the disintegrating drop wake is only hypothetical and much efforts is required for better understanding various processes inherent in the phenomenon.

One of the important observations of heterogeneous detonations is the fact of drastic improvement of detonation initiation when an appreciable portion of fuel is prevaporized [11, 12]. This can be attributed

to fast evaporation of the stripped sheet in the flow of ignited gaseous mixture and radial expansion of the wake cloud and better oxidizer entrainment in it.

Concluding Remarks

Current understanding of physical and chemical processes in heterogeneous detonations is based on the oversimplified treatment of various interactions between liquid-fuel drops with the shock-induced airflow. Energy release in heterogeneous detonations is simulated primarily as a one-dimensional phenomenon controlled by drop breakup time and some characteristic ignition delay time. Analysis of these interactions indicates that the encountered phenomena are very complex and inter-related. It is shown that the phenomena of drop breakup combined with the formation of a mixing layer of micromist droplets with air, micromist vaporization, ignition, and combustion exhibit many features that are not studied yet. The essential role is played by various local rather than averaged processes implying that a multidimensional treatment of the problem is inevitably required.

Acknowledgments

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References

1. Pilch, M. and C. Erdman. 1987. Use of break-up time data and velocity history data to predict the maximum size of stable fragments for acceleration induced break-up of a liquid drop. *Int. J. Multiphase Flow* 13:741–57.
2. Joseph, D.D., J. Belanger, and G.S. Beavers. 1999. Breakup of a liquid drop suddenly exposed to a high-speed airstream. http://www.aem.umn.edu/research/Aerodynamic_Breakup/
3. Reinecke, W.G., and G.D. Waldman. 1970. A study of drop breakup behind strong shocks with applications to flight. SAMS0-TR-70142. Avco Systems Division.

4. Frolov, S. M., V. Ya. Basevich, V. S. Posvianskii, and V. A. Smetanyuk. 2004. Vaporization and combustion of a hydrocarbon fuel drop. Part IV. Drop vaporization with regard for spray effects. *J. Advances Chemical Physics* 23(7):49–58.
5. Atthasit, A., N. Doue, Y. Biscos, G. Lavergne, and A. Berlemont. 2003. Influence of drop concentration on the dynamics and evaporation of a monodisperse stream of drops in evaporation regime. In: *Combustion and atmospheric pollution*. Eds. G. D. Roy, S. M. Frolov, and A. M. Starik. Moscow, Russia: TORUS PRESS. 214–19.
6. Joseph, D. D., A. Huang, and G. V. Candler. 1996. Vaporization of a liquid drop suddenly exposed to a high-speed airstream. *J. Fluid Mechanics* 318:223–36.
7. Borisov, A. A., P. V. Komissarov, A. V. Kulikov, O. I. Melnichuk, G. I. Skachkov, K. Ya. Troshin, and B. A. Khasainov. 1998. Kinetics of heat release in heterogeneous mixtures. *Chemical Physics Reports* 17(3):49–58.
8. Frolov, S. M., A. A. Scripnik, and R. Z. Kavtaradze. 2003. Modeling of Diesel spray ignition. In: *Combustion and atmospheric pollution*. Eds. G. D. Roy, S. M. Frolov, and A. M. Starik. Moscow, Russia: TORUS PRESS. 220–27.
9. Scripnik, A. A., S. M. Frolov, R. Z. Kavtaradze, and V. V. Efros. 2004. Simulation of ignition in a liquid fuel spray. *J. Advances Chemical Physics* 23(1):54–61.
10. Frolov, S. M., V. Ya. Basevich, V. S. Posvianskii, and A. A. Belyaev. 2004 (in press). Drop vaporization and combustion with spray effects. In: *Combustion and pollution: Environmental impact*. Eds. G. Roy, S. Frolov, A. Starik. Moscow, Russia: TORUS PRESS.
11. Benedick, W. B., S. R. Tieszen, R. Knystautas, and J. H. S. Lee. 1991. Detonation of unconfined large-scale fuel spray–air clouds. In: *Dynamics of detonations and explosions: Detonations*. Eds. A. L. Kuhl, J.-C. Leyer, A. A. Borisov, and W. A. Sirignano. Progress in astronautics and aeronautics ser. New York, NY: AIAA Inc. 133:297–310.
12. Frolov, S. M., V. Ya. Basevich, and V. S. Posvianskii. 2004. Limiting drop size and prevaporization degree required for spray detonation. In: *Application of detonation for propulsion*. Eds. G. D. Roy, S. M. Frolov, and J. E. Shepherd. Moscow, Russia: TORUS PRESS. 110–19.