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Review

Physical and Mathematical Models of Micro-Explosions: Achievements and Directions of Improvement

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Abstract: The environmental, economic, and energy problems of the modern world motivate the development of alternative fuel technologies. Multifuel technology can help reduce the carbon footprint and waste from the raw materials sector as well as slow down the depletion of energy resources. However, there are limitations to the active use of multifuel mixtures in real power plants and engines because they are difficult to spray in combustion chambers and require secondary atomization. Droplet micro-explosion seems the most promising secondary atomization technology in terms of its integral characteristics. This review paper outlines the most interesting approaches to modeling micro-explosions using in-house computer codes and commercial software packages. A physical model of a droplet micro-explosion based on experimental data was analyzed to highlight the schemes and mathematical expressions describing the critical conditions of parent droplet atomization. Approaches are presented that can predict the number, sizes, velocities, and trajectories of emerging child droplets. We also list the empirical data necessary for developing advanced fragmentation models. Finally, we outline the main growth areas for micro-explosion models catering for the needs of spray technology.

Keywords: heterogeneous fuel droplets; micro-explosion; puffing; critical conditions; parent and child droplets; modeling

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1. Introduction

A micro-explosion is the rapid secondary atomization of droplets composed of at least two liquids with widely different boiling temperatures [1–3]. As a droplet is heated by the ambient air, one liquid boils at the core of it, while the other one envelops it to confine the emerging bubbles within the droplet. As a result, the vapor bubbles fill the droplet and then coalesce into a single vapor buffer layer. Once the bubble grows to a critical size and the film around it reaches a critical thickness, the film breaks up into an aerosol of secondary droplets [4–6], several orders of magnitude smaller in size than the original droplets [7–9]. The lower the boiling temperature of one of the liquids in the droplet, the less energy is spent on its heating to a micro-explosion. This makes water a popular component in heterogeneous droplets. Active research is currently focused on parent droplets of water-based solutions, slurries, and emulsions, including micro- and nano-emulsions [9–12]. It involves different heating arrangements with dominant convective, conductive, radiative, and mixed heat transfers [13–16] to determine the critical conditions sufficient for the parent droplet breakup and the limitations to the use of these effects in various engineering systems.

Numerous experiments have incorporated tracking software and hardware based on high-speed cameras and laser diagnostic systems [4,17–19] and shed new light on the necessary and sufficient conditions for the micro-explosive breakup of heterogeneous droplets. Unique data were obtained about vaporization centers in the form of the sub-droplets of one liquid embedded in the other [20–22], solid particles [23–27], gas and

vapor bubbles [28–31], and liquid–liquid interfaces of different geometries [22,32]. Several research teams focused on the integral characteristics of the secondary droplets (also referred to as child droplets) produced from the breakup of parent droplets [4,15,23,33,34]: their number, size, total surface area, velocities, trajectories, and compositions. These authors also obtained approximations for predicting the values of these characteristics depending on the heat flux, parent droplet size and compositions, etc. [4,15,23,33,34]. In recent years, these findings have accelerated the development of physical and mathematical models describing micro-explosive droplet fragmentation.

Widely known in-house codes written in Matlab and Mathematica [35–40] as well as models developed in commercially available packages (Ansys Fluent, Comsol Multyphisics, OpenFoam) [41–46] are used for calculating the integral characteristics of a droplet micro-explosion. These models are based on the theories of heat and mass transfer, chemical physics, fluid dynamics, molecular dynamics, etc. Whether a model is applicable to each specific case is defined by the micro-explosion criteria (necessary critical conditions) as well as the known input parameters. The latter are often determined experimentally and used as empirical data for the numerical solutions to micro-explosion problems. Limits to the applicability of known micro-explosion models motivate scholars [47] to improve them by enhancing their capability to predict droplet breakup behavior in applications that involve liquid spraying [10,48–53].

Micro-explosive breakup is classified as a secondary atomization approach [30,54–56]. Other approaches for secondary droplet atomization include droplet–droplet collisions in a gas, droplet impingement on solid walls, and droplet collisions with gas flows. Antonov et al. [57] established that micro-explosions can increase the liquid surface area by an order of magnitude more than any other secondary atomization systems can. This is a major prospect for heat exchange, evaporation, fuel, medical, petrochemical, and other technologies. Here, a micro-explosion is provided by synergistic cascade effects (child droplets break up after parent droplets do) in plants and reactors, thus improving their overall performance [58–62].

It is important to generalize and compare findings obtained by different research teams to understand the latest achievements in modeling interconnected physicochemical processes occurring during the heating, evaporation, and micro-explosion of liquid droplets. Tackling these problems using numerical simulations, analytical solutions, empirical approaches, experimental research, prototype tests, and combined methods often yields new scientific knowledge about complex phenomena and processes. In writing this review, we were motivated by the need to summarize the state of the art in physical and mathematical models simulating micro-explosions. The aim of this work was to identify the best solutions to the pressing problems in modeling micro-explosions of different-size composite fuel droplets and to suggest promising areas for further research in the field of fuel technology. The initial size of the parent droplet is a major factor. It defines the micro-explosion dynamics and, hence, the limitations to the applicability of specific models for predicting the characteristics of this process. Clearly, models describing droplet micro-explosion for different applications boost the use of artificial intelligence and computational methods in these applications. In particular, these models make it possible to develop unattended automatic control systems for the spraying, atomization, mixing, coalescence, and separation of components in multiphase gas–vapor-droplet flows. The critical conditions and characteristics of droplet micro-explosions heavily depend on the input parameters (for instance, ambient temperature, heat flux, droplet size and composition, etc.). Therefore, these conditions should be optimized towards minimizing breakup delay or maximizing the number of secondary fragments by means of artificial intelligence algorithms using effective values of parameters selected from a large database. Advanced research centers in Europe, the USA, Japan, China, India, Russia and other countries annually contribute to this database by adding their numerous experimental findings. Practical applications require multiple droplet micro-explosions under the same conditions, in cycles or cascades, in line with industrial processes, so it is important to use neural networks. It is especially

important to optimize the processes involved in the cascade micro-explosions of parent droplets and all child droplets in the form of echelons.

2. The Phenomenon of Micro-Explosion

The first mentions of a micro-explosion (Figure 1) date as far back as 1962 [1]. However, the scientific field associated with the micro-explosive breakup of droplets, films, layers, and sprays has gained new momentum due to improved high-speed cameras for studying fast-paced phase transitions. A micro-explosion is commonly defined as the fast-paced breakup of a parent two-liquid or emulsified droplet triggered by the superheating of internal water droplets above their boiling point [1,22]. The droplet breaks up into a large number of small secondary fragments, from dozens to hundreds of micrometers in size. The most typical liquids used for micro-explosive effects are as follows: water as a chemically inert low-boiling liquid and diesel fuel (or dodecane), kerosene (or decane), and biodiesel (or rapeseed oil) as combustible high-boiling liquids. Figure 2 shows typical images of experiments with the micro-explosion of a two-liquid droplet.

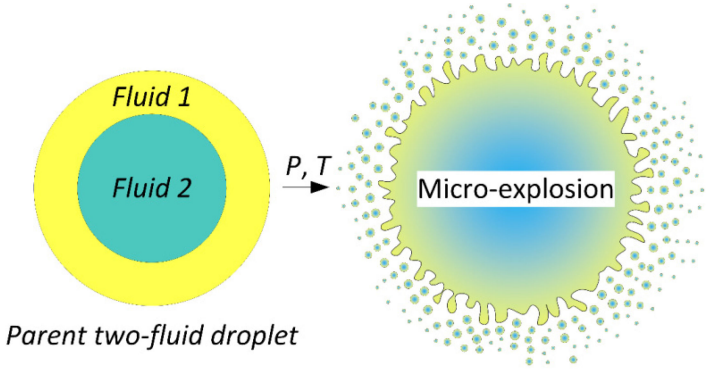

Figure 1. Schematics of micro-explosive breakup.

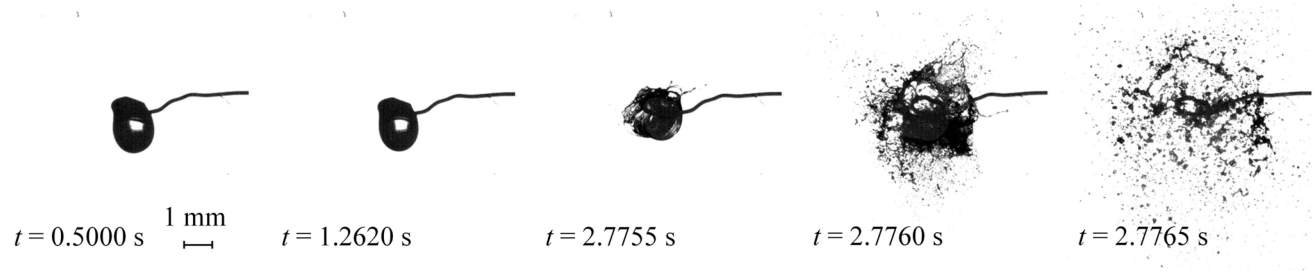

Figure 2. Micro-explosive breakup of water/kerosene droplets ($R_{d0} \approx 1.3$ mm, $\eta_f \approx 80\%$, $T_a \approx 773$ K).

Figure 3 shows another breakup regime—puffing—where nucleation is limited to a portion of the droplet [17,63,64]. The bubbles do not usually coalesce with their neighboring counterparts. That is why they leave the droplet faster but do not trigger its disruption. As the bubbles implode, large parts (over 100 μm in radius) detach themselves from the droplet. A higher ambient gas temperature or increased combustible liquid concentration in a droplet provokes a transition to the micro-explosion regime, where a droplet is superheated, and rapid bubble nucleation occurs throughout the droplet.

The most interesting findings on micro-explosive breakup have been obtained for immiscible two- and three-liquid droplets [40,65], emulsions [6,17,66], slurries [55,67–69], and solutions [62,70–73]. The concentration of the combustible and non-combustible components has a strong impact on the micro-explosive breakup [74]. Although the thermal diffusivity of water is much higher than that of the liquid combustible components, the latter evaporate faster because the heat of their phase transition is several times lower. As a result, liquid combustible components are heated above the water boiling point within a short time. Here, the droplet breakup delay largely depends on how fast water reaches

its boiling point. The lower the proportion of water in a composite fuel droplet, the sooner this happens. However, there must be enough water for a water–fuel interface to form, as this will provide a large number of secondary droplets.

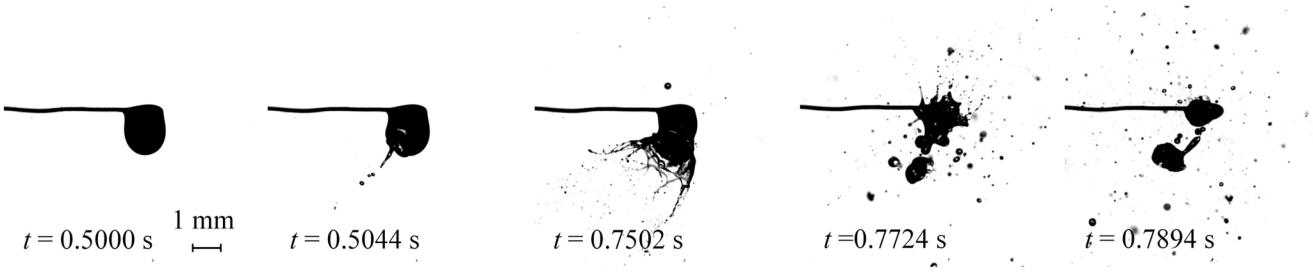

Figure 3. Puffing of water/rapeseed oil droplets ($R_{d0} \approx 1.3$ mm, $\eta_f \approx 80\%$, $T_a \approx 773$ K).

The droplet breakup (micro-explosion) mechanism (Figure 4) relies on bubbles filled with vapors of superheated liquid emerging at the water–fuel interface [3,75–77]. As they grow in size, coalesce, and move into a two-liquid droplet, the pressure inside them increases. As soon as it exceeds the pressure of the surface tension forces acting on the droplet, the droplet breaks up. If the gas pressure in the bubbles increases fast enough, the parent droplet will explode to form secondary droplets (micro-explosion). If it increases slowly, different-size secondary fragments will detach themselves from the droplet (puffing). The more dissimilar components a droplet contains, and hence the greater the number and total area of interfaces in it, the more effective its fragmentation. At the same time, such heterogeneities (especially in high concentration) reduce the vapor pressure in a droplet and increase the duration of the breakup in general. Figure 4 presents a physical model of two-liquid droplet fragmentation (in stages). First, vapor bubbles nucleate at the water–fuel interface. Then, the bubbles proceed through the combustible liquid film. Finally, the water and combustible liquid fragments (child droplets) detach themselves from the parent droplet.

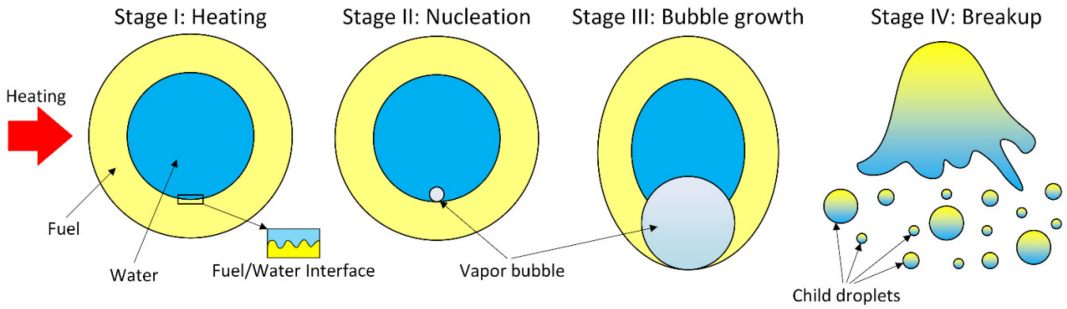

Figure 4. Physical model simulating the micro-explosive breakup of a two-liquid droplet into secondary fragments.

The typical conditions have been identified for a more extensive micro-explosion of multi-component and multi-phase droplets [4,22,43,54]. The authors developed in-house test benches and used them to experimentally obtain relationships between the heat and mass transfer characteristics in the system of a heterogeneous droplet/high-temperature ambient gas and a set of the main parameters. These parameters include the temperature of the heating environment (300–1500 K), the heating arrangement (heated air flow, heated substrate, muffle furnace, or burner flame), the flammable liquid concentration (3–97%), viscosity (0.00259–0.01668 Pa·s), the interfacial tension (0.00341–0.04257 N/m), the surface tension (0.0401–0.07269 N/m), the material (water, kerosene, diesel fuel, transformer, and rapeseed oil), the droplet size (0.5–1.5 mm), and the preparation technology (two-liquid droplets and emulsified fuels), as well as combined effects. The findings can help to reduce

the time and energy needed to intensify the corresponding heat and mass transfer processes in high-potential applications.

Previous research has shown that the micro-explosions of liquid, slurry, and emulsion droplets at the heating stage can increase their evaporation area by up to 15 times [78–80]. However, it has yet to be determined how much the evaporation area may increase depending on the mechanism used to supply energy to the droplet surface: using conductive, convective, radiative, or mixed heat transfer. As shown by PLIF experiments [81], the heating and evaporation rates vary considerably when a droplet is exposed to conductive, convective, radiative, or combined heat transfer. Conductive heat transfer provides the highest water droplet heating rates (up to 100 K/s), while the lowest ones (up to 30 K/s) are observed during radiative heat transfer. The highest water droplet evaporation rates (up to 0.07 kg/(m^2·s)) are recorded when the droplet is exposed to convective heat transfer, and the lowest ones (up to 0.025 kg/(m^2·s)) during conductive heat transfer. As a result, the heating, evaporation, and atomization behaviors and outcomes differ greatly as well. The evaporation dynamics of liquid droplets in the course of their breakup so far remains understudied. The evaporation intensity depends on the temperature at the phase transition surface and on the concentration of liquid vapors next to the interface. The evaporation is driven by the diffusion and heat transfer in this area. No experimental data on local heat and mass transfer near the surface of evaporating droplets have been published so far; the underlying physical mechanisms have not been described either.

3. Progress in Mathematical Modeling

Today, most of the well-known models of droplet micro-explosions in a gas are based on ad hoc numerical methods implemented in commercially available software products (Ansys Fluent, Comsol Multiphysics, OpenFoam, SigmaFlow, etc.). Many scholars use direct numerical simulations [3,8,43,62,82–84] and in-house sub-models based on analytical solutions [38,85–87]. Several hypotheses [3,27,38,43,62,88,89] have been formulated about the physical patterns of a micro-explosive breakup. Shinjo et al. [3] presented a comprehensive approach to modeling the micro-explosion of a fuel emulsion droplet. They showed that this process largely depends on the explosive boiling of embedded water sub-droplets as well as liquid–vapor interface oscillations. They observed bubble nucleation near the water–fuel interface, i.e., at the surface of water sub-droplets. The micro-explosion of emulsion droplets is affected by the distribution of dispersed water sub-droplets, their initial size, and their coalescence triggered by thermocapillary convection [3]. The models described in [27,38] can estimate the heated droplet micro-explosion delay using the analytical solution of the heat conduction equation inside a two-liquid droplet. A temperature distribution inside a two-liquid droplet is obtained at every time step of the solution process; the criterion for micro-explosion is based on the water nucleation temperature reached at the water–fuel interface [27,38]. Micro-explosion delays depend on the gas flow temperature as well as the concentration and size of solid particles in the water [27]. A model has been proposed for predicting the temperature distribution inside an emulsion droplet under convective heating, reflecting the angular dependence of the effective conductivity and the eccentricity of the temperature field [43]. The temperature distribution inside an emulsion droplet significantly affects the initiation of puffing/micro-explosions, i.e., water nucleation. Shinjo et al. [43] proved that the shear force due to the heated gas flow causes internal circulation inside a droplet. In their experimental research on micro-explosions in diesel fuel and ethanol blends, Avulapati et al. [62] hypothesized that micro-explosions result from the superheating and rapid evaporation of ethanol in the blend. They also concluded that a higher pressure enhances the micro-explosion. This can be an argument in favor of using these effects in diesel engines [62]. One of the first unified models simulating the micro-explosion of emulsified droplets was presented by Fu et al. [89]. The authors [89] made the following conclusions as to the mechanism of a micro-explosive breakup: (i) the condition for a micro-explosion is that the temperature of the droplet reaches the superheat limit of the embedded water; (ii) nucleation is heterogeneous and requires a much

lower superheat limit than with homogeneous boiling; (iii) the effect of surface tension on superheat is negligible. For a micro-explosion to occur, an oil membrane must be formed around the droplet, which leads to the superheating of the internal water. The criterion for a micro-explosive breakup is the critical thickness of the oil membrane around the droplet, enabling water to reach the superheat temperature [89]. A series of experiments has proved [90] that micro-explosions follow the formation of one or two bubbles near the droplet core due to the superheating of the low-boiling component (most often water). According to a study by Li et al. [91], the bubble nucleation in a droplet with its subsequent breakup depends on the rate of superheating. Antonov et al. established [92] that a droplet breaks up because bubbles expand inside of it, and its surface tension decreases due to superheating. One of the first and relatively simple micro-explosion models was based on the criterion of the water–fuel interface superheating above the boiling point [93]. As the heat transfer intensifies, the low-boiling component (water) concentrates in the droplet core and is heated to the temperatures needed for nucleation to occur. This is a necessary condition of droplet fragmentation [93].

Popular current models of micro-explosive breakup, for instance [3,43,88,89], have a number of limitations because their numerical results largely depend on the input experimental data. Such data are unavailable for some processes and thus render them ineligible for modeling. Shinjo et al. [3] used a statement where water inside an emulsion droplet is superheated at the initial moment in time and there is a vapor bubble in it (so, the micro-explosion conditions are reached). The authors showed that, with this problem statement, the calculations depend heavily on the initial conditions: the initial radius of the water sub-droplet and the location of the water sub-droplet in the fuel, as well as the location of the vapor bubble inside the water sub-droplet [3]. This approach describes the emulsion droplet destruction as it reaches the micro-explosion conditions, but it does not elucidate the processes occurring in a droplet being heated. The model described by Shinjo et al. [43] can predict the temperature distribution inside an emulsion droplet and, hence, the locations of future vaporization centers in dispersed phase droplets, but it does not provide insight into the breakup of such droplets. In the unified model by Fu et al. [89], the micro-explosion criterion is that an oil membrane of a critical thickness is formed at the droplet surface. The criterion depends on the initial droplet size, dispersed phase size, and volume fraction of water in the emulsion and implies that no micro-explosion occurs in droplets under 100 μm, but contemporary studies of micro-explosions in diesel engines [94,95] do not corroborate this hypothesis. No universal model of a two-liquid droplet micro-explosion has yet been developed due to specific bottlenecks (mostly discussed by Sazhin et al. in [93]), including the links between breakup mechanisms and outcomes. For these reasons, we see high potential in theoretical research into the heating, evaporation, swelling, micro-explosion, and further ignition of liquid droplets using the best-known criteria [3,43,62,88,89]: superheating of the water–fuel interface above the boiling point, reaching the critical bubble size before breakup and exceeding the critical pressure in the vapor film. Figure 5 presents typical schematics for describing the processes involved in micro-explosion [3,27,38,89] (the statements are case-specific).

Here we should outline several important physical aspects of the heterogeneous droplet transformation upon heating before a micro-explosion. These physical aspects have been demonstrated in detail in experimental findings [2,21,22]. First, the structure of an emulsion droplet shown in Figure 5c quickly transforms into what is shown in Figure 5a upon heating. This results from the intense coalescence of water droplets due to thermogravitational convection as well as reduced viscosity, surface tension, and interfacial tension. The higher the ambient gas temperature, the faster the droplet structure transitions from Figure 5c to Figure 5a. Generalized findings [2,21,22] indicate that an emulsion droplet rapidly stratifies when it reaches 40–60 °C, depending on the composition and properties of the emulsifier used in the experiments. The time it takes a droplet to transition from Figure 5c to Figure 5a usually does not exceed 5% of the droplet micro-explosion delay time. That is why the simplified statement from Figure 5a is applicable for modeling

droplet micro-explosions at elevated ambient gas temperatures. The second aspect is related to the initial location of the water core and vapor bubble in a heterogeneous droplet (Figure 5b). According to research findings [96–98], water droplets are displaced from the center of the parent droplet to its lower surface due to different densities of water, the combustible component (for instance, rapeseed oil, diesel fuel, kerosene, or gasoline), and thermogravitational settling. Vapor bubbles nucleate near the fuel–water interface due to water superheating to its boiling point. Water cannot stay in a metastable state inside a droplet for a long time: the balance of pressures, energies, and forces is difficult to maintain. Vapor bubbles form and rapidly leave the droplet, breaking it up in the process. The droplet breakup front emerges near the thinnest fuel film around the vapor bubble. This aspect should be taken into account when using the statement from Figure 5c, otherwise the predicted droplet breakup delays can differ quite substantially from the experimental data. The third aspect is related to the shape of the parent droplet and its placement in the heating area. The current models most often use a spherical droplet shape. They simulate a droplet hovering in a gas, but the droplet holder or the oncoming, often turbulent, gas-air flow are usually not modeled. However, this is what holds a droplet in a heated environment in most of the experiments [99–101]. So, if there are significant differences between droplet micro-explosion delays predicted by advanced models and those obtained experimentally, neglecting to research the object arrangement could be the reason. This factor becomes especially important if the experiments involve holders of different shapes (rod, loop, substrate, etc.) and materials (metal, ceramics, etc.).

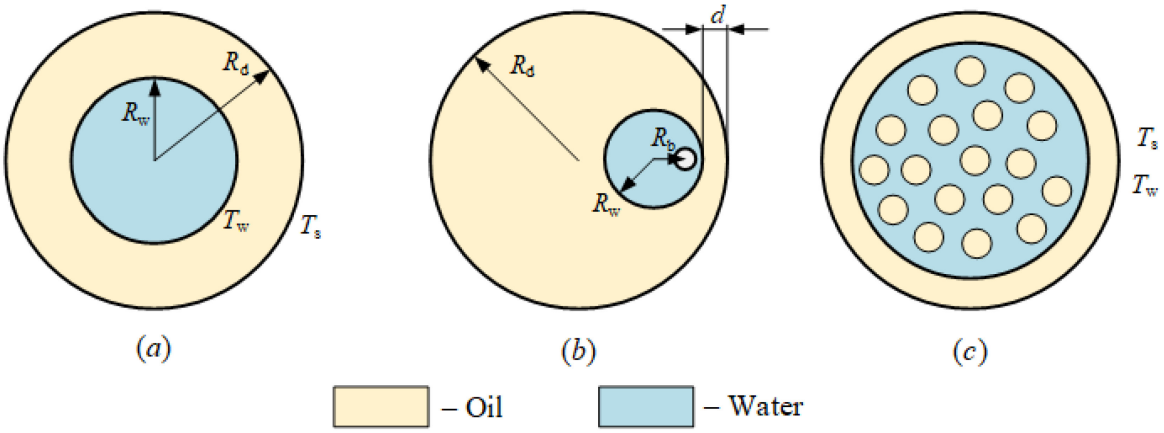

Figure 5. Typical schematics for describing micro-explosion: (**a**)—[27,38], water droplet of radius R_w inside a fuel droplet of radius R_d, T_w is the temperature at the water–fuel interface, T_s is the temperature at the droplet surface; (**b**)—[3], emulsion droplet geometry; (**c**)—[89], oil membrane forming in an emulsion droplet.

We believe that the industry would greatly benefit from detailed models of two-liquid droplet breakups from the beginning of heating up to disintegration, starting simple and gradually becoming more complex [96–98]. A specific case of tackling this problem can be based on a statement, in which the temperature at the water–fuel interface is at the nucleation point, and there is a vapor layer (2) of thickness δ with an inner pressure equal to the pressure of saturated vapors, P_v, around the water core (1). Figure 6 schematically shows the solution space for this problem. The parameters δ and P_v can be assumed free and variable for adjusting the model and defining the physical mechanisms of a droplet breakup and the transitions from one regime to another. Free parameters have a well-grounded variation range. For the film thickness, δ, this range varied from zero to two-three times the droplet radii, according to the experimental observations [8,24,82,102], and saturated vapor pressure varied from zero to the liquid-specific critical values. A complex statement should also reflect phase transitions.

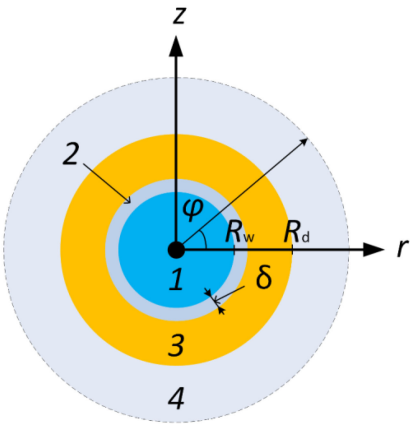

Figure 6. Schematic solution space (1—water; 2—water vapor; 3—fuel; 4—air); R_w is the water core radius; R_d is the droplet radius.

We propose to use the Volume of Fluid (VoF) method for this problem. In the VoF method, advection equations are solved for the volume fractions of the present phases, α_i, provided that $\sum_{i=1}^{4} \alpha_i = 1$. The interfaces are approximated by smooth functions controlled by numerical dissipation to preserve the thin transition area. Velocity, temperature, and pressure fields are the same for all the phases present. The continuity, momentum, and energy equations are solved for the effective fluid, whose properties depend on the local volume fractions of each phase. In addition to a Navier–Stokes system of equations, it is necessary to solve the advection equations for the volume fractions. Below is the mathematical formulation of the problem (using the VoF method) [103].

Physical properties of each i-th phase are described by the equations of state:

$$\rho_i = \rho_i(P, T),\ h_i = e_i(T) + \frac{P}{\rho_i},\ \mu_i = \mu_i(T),\ \lambda_i = \lambda_i(T),$$

where ρ is the liquid density, h is specific enthalpy, e is specific internal energy, μ is dynamic viscosity, λ is thermal conductivity, and i is the phase number.

The properties of the system components are written as

$$\rho = \sum_i \alpha_i \rho_i,\ h = \rho^{-1} \sum_i \alpha_i \rho_i h_i,\ \mu = \sum_i \alpha_i \mu_i,\ \lambda = \sum_i \alpha_i \lambda_i.$$

Continuity equations for all the phases take the form

$$\frac{\partial \rho_i \alpha_i}{\partial t} + \nabla(\rho_i \alpha_i U) = 0.$$

where t is time, and U is velocity.

Figure 7 illustrates the simulation of different-scale droplet fragmentation. At the first stage, we can observe the typical disruption of a vapor film into smaller parts (vapor bubbles). Then the vapor bubbles entrain water and fuel, thus forming secondary fragments. The breakup dynamics and regimes largely depend on the saturated vapor pressure in a vapor film, its thickness, and properties of the fuel envelope (density, viscosity, and surface tension).

Models predicting the number, size, velocities, and trajectories of secondary fragments are not often used in the process environment [43,62,82]. Such models heavily depend on empirical data, and their results for sprays are averaged from those for single droplets. It is difficult to model two or more droplets breaking up to form a fine spray, especially in the case of a cascade breakup. To accurately reproduce the formation of a spray from each parent droplet, it is necessary to describe its heating, surface transformation, heat and mass transfer, phase transitions, micro-explosion, and other processes. In this respect, it seems

promising to discover several basic scenarios of parent droplet behavior given the known experimental data. These scenarios can then be transferred to child droplets, which become the new micro-explosion centers upon heating, i.e., serve as parent droplets. The setting for these scenarios should be combustion chambers, reactors, and other systems with superheated heterogeneous droplet flows, controlling for temperature and concentration fields, heat fluxes, and aerodynamic aspects.

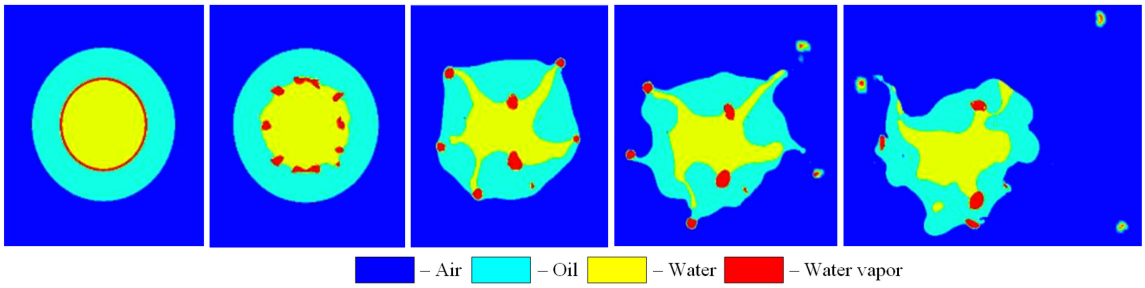

Figure 7. Typical outcomes of different-scale droplet fragmentation (R_{d0} = 1.3 mm, R_{v0} = 0.8 mm, R_{w0} = 0.75 mm, water/rapeseed oil, combustible liquid concentration 80%, vapor layer thickness 0.05 mm, initial pressure in the vapor layer 10^6 Pa).

Models based on the Volume of Fluid (VoF) method [103] can receive major impetus if the changing structure and composition of a parent droplet upon superheating are accurately identified in experiments. Such experiments will require high-speed video recording, laser diagnostics, and adaptive tracking of moving objects: planar laser-induced fluorescence (PLIF) [28,80,104–107], laser-induced phosphorescence (LIP) [108], particle image velocimetry (PIV) [109], interferometric particle imaging (IPI), and shadowgraphy [110]. When used in combination, these methods can reproduce the structure of a parent droplet in different sections and identify dominant and auxiliary thermal, physicochemical, and fluid dynamic processes. The results obtained using a combination of these methods have shown that the composition of secondary fragments can be changed in a controlled manner by varying the values of the main input parameters: the heating arrangement and heat flux, the initial size of parent droplets, and the relative concentration of water and fuel in them.

A comparative analysis of mathematical modeling results and experimental data [8,24,82,102] have shown that the initial size of a parent droplet plays the principal role in the breakup model selection process. Droplet shape heavily depends on its size: the larger the initial droplet, the less spherical it is. It takes the shape of an oblong or oblate ellipsoid along the direction of its movement. The micro-explosion delay of non-spherical droplets can only be reliably predicted from experimental data at the location of water and vapor bubbles in those droplets. The smaller the initial droplet, the less reliant the model is on the empirical data from experiments. Droplets of less than 100 μm can be assumed to have a stable spherical shape and a fuel film of even thickness around the water and vapor bubble. The relative positions of parent droplets in a spray should also be taken into account. Experiments by Antonov et al. [111] revealed the combined effects of parent droplets in sprays on their micro-explosive behavior. It was established that if the distance between parent droplets exceeds 8–10 times their typical radii, the distributions of secondary droplets from each parent droplet are virtually identical. Only in the case of this rarefied initial spray, a single parent droplet model can be used to predict the breakup conditions and outcomes for an array of droplets in a flow. However, if parent droplets are arranged more densely in the gas-air flow, they collide both with each other and with child droplets, so their collective effects on heating and surface transformation should be taken into account. The higher the ambient gas temperature and the denser the seeding of parent droplets, the more substantial these effects are.

Research findings [5,112] show that the heating arrangement of initial droplets has a decisive effect on the number and size of secondary fragments produced in the puff-

ing and micro-explosion regimes. The maximum number of secondary fragments was recorded [5,112] in experiments where parent droplets were placed on a heated solid surface (with dominant conductive heat transfer), and the minimum number of droplets were produced upon heating in a tubular muffle furnace (with dominant radiative heat transfer). In experiments with dominant convective heat transfer, the authors recorded the average number of secondary fragments compared with other arrangements studied [5,112]. The aspects outlined in the experiments [5,112] can benefit the mathematical models of droplet breakups by controlling for critical heat fluxes at the droplet surface in contact with the heating environment.

4. Applications Involving Micro-Explosive Breakup

The evaporation of two-liquid droplets, emulsions, slurries, and solutions is widely used in many applications [21,78–80,113–116]: combustion of liquid fuels in engines and heat-generating plants, separation of emulsions and slurries into individual components (evaporation, drying, and burnoff), thermal wastewater treatment, fire suppression using specialized blends, etc. Droplet evaporation can be significantly intensified by dispersing the flow with the help of atomizers, nozzles, adapters, grids, etc. With two-liquid droplets, however, there is the option of using micro-explosion as a way to accelerate evaporation and improve its efficiency. As a rule, research teams study such effects at the request of car manufacturers in pursuit of higher performance (for example [21,78–80,115,116]). Figure 8 shows typical applications involving micro-explosive breakup.

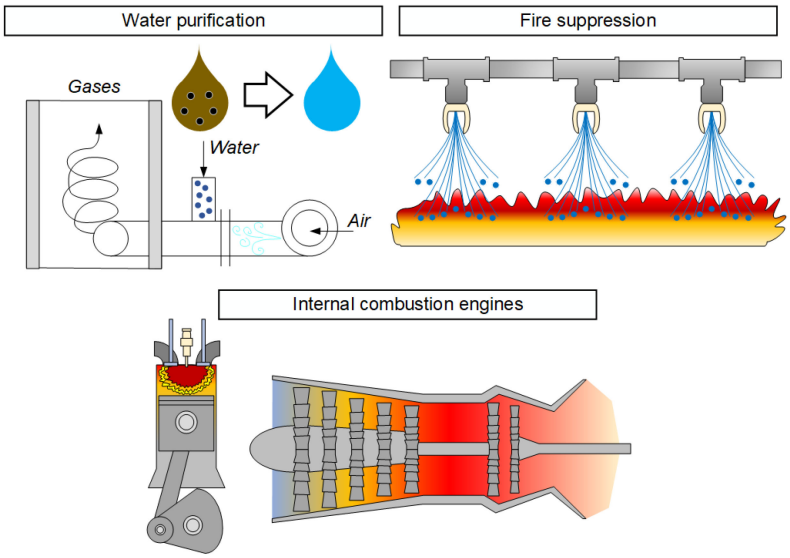

Figure 8. Potential applications of micro-explosive breakup.

With the growing environmental problems worldwide, biofuels based on plant-derived oils are becoming more popular in the energy and transportation industries. The use of biofuels as an alternative to conventional fossil fuels effectively reduces the emissions of carbon, nitrogen, and sulfur oxides [117]. One of the most promising strategies for emission reduction is switching to renewable energy sources (plant-based fuels in particular: biodiesel, biokerosene, bioethanol, and biogasoline) [118,119]. The micro-explosions of two-liquid droplets can make biofuel production more effective. They provide a several-fold increase in the liquid evaporation surface area through breaking up parent droplets into fragments that can be dozens of microns in size [120,121].

Breakthroughs in thermal wastewater treatment using an atomized flow can only happen if we know the physical principles underlying the behavior of the water solution, emulsion, and slurry droplets traveling through high-temperature gases, such as air and fuel combustion products. There is no theory of heat and mass transfer and phase transformations for such conditions at this point. However, some recent experimental findings

(for example, [122–124]) have provided fertile ground for developing one. Comprehensive research findings are lacking because these processes are difficult to model; there are many interfaces with highly nonlinear boundary conditions for nucleation. These difficulties have been outlined in a review paper [96] among the barriers to modeling the rapid heating and evaporation of fuel and emulsion droplets.

Many recent studies have focused on micro-explosive breakups in internal combustion engines [94,125]. The use of water-in-fuel emulsions as an alternative to conventional fossil fuels in diesel engines solves two problems at once: the fuel energy is used more effectively and anthropogenic emissions are reduced. For instance, the micro-explosion of emulsified fuel droplets in diesel engines significantly improves the fuel combustion efficiency due to secondary droplet atomization [89,126]. Moreover, water added to the fuel composition reduces NO_x emissions by up to 60% and fuel consumption by up to 21% [95]. Similar trends have been established for gas turbine engines. Adding even a small amount of water (3–12%) to aviation kerosene makes it possible to significantly reduce nitrogen oxide emissions in certain ranges of engine power [127,128]. Micro-explosions can be actively used in firefighting, where the surface area of the liquid in the combustion zone increases significantly due to this effect [120].

It is important from a practical standpoint to transition to the use of micro-explosions in power plants, airplane engines, ground-based power systems, etc. This will require the following: (i) creating a database with the characteristics of the secondary fragments produced by the micro-explosions of a small array of neighboring parent droplets arranged in a spray (the experimental methods and setups should be adjusted to identify the composition, size, velocity, and other characteristics of secondary droplets); (ii) developing probabilistic models simulating the micro-explosions of droplets in sprays while controlling for coalescence, bounce, separation, and the disruption of neighboring parent and child droplets.

5. Conclusions

This review has outlined the most interesting mathematical models of micro-explosions developed by research teams from different countries using advanced software and hardware systems. The critical (necessary and sufficient) conditions of droplet micro-explosions are described using models based on calculations of the threshold temperature at the fuel–water interface, the temperature gradient at this interface, the critical size of the vapor bubble, and the minimum thickness of the liquid film around it. The models are based on analytical approaches, in-house computer codes calculating the coupled heat and mass transfer, as well as commercial packages using discrete numerical simulations. All these models have become possible due to new insights into the physics of heating, evaporation, micro-explosion, and the ignition of heterogeneous fuel droplets. New challenges have been determined that need to be tackled to improve the numerical simulation of micro-explosions. The ones that are relevant to the widest application range are grouped as follows: (1) developing universal complex models of heat and mass transfer, fluid dynamics, chemical physics, molecular dynamics, and other theories to describe the critical conditions for the breakup of parent droplets (superheating of the liquid–liquid interface, vapor bubble growth, and thinning of the liquid film around the vapor phase); (2) developing models describing the production and distribution of the secondary fragments when the micro-explosion criteria are met; (3) developing predictive models describing the cascade and collective effects of the micro-explosive breakup of parent and child droplets in sprays; (4) developing models that can predict the composition of sprays produced by the micro-explosion of liquid droplets.

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