Cumulative effect in foams and mechanism of detonation development

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Abstract. The paper is devoted to the analysis of non-steady combustion and detonation in aqueous solutions foamed with the hydrogen-oxygen gaseous mixture. The processes of flame acceleration and transition to detonation are studied experimentally and numerically. Based on complex analysis, the effect of cumulative compression of the reactive gaseous mixture inside collapsing bubbles is proposed to be the mechanism of detonation formation and its further self-sustained propagation. Flame propagation through the foam leads to the compression waves generation. Under the action of compression waves, the gas bubble collapses, and states with high energy densities are achieved inside the bubble. As a result, the ignition inside the bubble takes place that represents a basic mechanism of detonation formation and propagation.

1. Introduction

Porous media and the foams, represent a vivid example of the system in which the development of dynamic processes is associated with the generation of the states with high energy densities [1]. Herewith, the aqueous foams are of particular interest. As it was shown in [2], the addition of combustible components to the composition of the foam makes such foams combustible. Moreover, at high enough reactivity of the combustible components, the combustion would develop via a non-steady way and can lead to the detonation onset. Such a regime with a transition to detonation was observed recently in the wet aqueous foams prepared via bubbling with a hydrogen-oxygen mixture [3, 4]. Such a system differs from the water-containing two-phase combustible systems studied earlier, such as bubbly liquids [5] and dry foams bubbled with premixed combustion mixtures [6–8]. At the same time, wet foams possess intermediate parameters between bubbly liquids and dry foams. So, it is reasonable to expect that the mechanisms of flame acceleration and transition to detonation can be rather close to those realized both in dry foams and bubbly liquids.

As the experience shows, the flame acceleration and transition to detonation in many ways are related to the phenomenon of energy cumulation. Thus, for example, the transition to detonation is much more plausible to take place in confined vessels rather than in unconfined spaces [9]. Moreover, more violent regimes of flame acceleration are usually observed in obstructed channels [10] or inside porous mediums [11]. The effect of geometrical confinement limits the scattering of energy released in the chemical reaction that leads to the formation of directed reacting flow, which intrinsically accelerates. The acceleration, in turn, leads to the formation of the shock waves and finally, the detonation onset can take place. A quite close mechanism is responsible for detonation onset in dry foams, where the single large bubble plays a role of such a closed volume, and transition to detonation develops on the scales of
this single bubble [8]. When transmitting from one bubble to another, the detonation wave decays, and then the process of flame acceleration and transition to detonation repeats in the neighboring bubble. In such a way, the detonation propagates through the dry foam with the help of a cumulation effect. When studying bubbly liquids [5], one cannot observe the formation and development of the flame in a medium containing such a large amount of water. However, a strong shock wave can provide the conditions required for detonation formation. Herewith, the magnitude of the shock wave can be relatively low compared to that causing detonation formation in the pure gaseous mixtures, and the leading role in the detonation sustenance belongs to the cumulation effect. After the compression by the shock wave, each bubble begins to collapse. As a result, the combustible mixture inside the bubbles is axially compressed, which leads to the mixture ignition after a certain time delay. Multi-bubble ignition causes enhancement of the decaying shock wave, and the process propagates further.

In the wet foam, it was experimentally observed [3] that the stage of flame development is plausible in such a medium distinct to the bubbly liquid. At the same time, the intensity of the leading shock wave is relatively low, and, presumably, the cumulation mechanism becomes to play a certain role. So, at first blush, the combustion development in the wet foam demonstrates the intrinsic features of combustion in both dry foams and bubbly liquids. Given this, here it is proposed to analyze in more detail the process of flame acceleration and transition to detonation in the wet foam that should provide more detailed insight into the combustion and detonation development in multiphase systems.

2. Problem setup

Microfoam was prepared on the base of aqueous solution with or without the addition of heptane droplets (of ~40 µm diameter) inside the tube of 3.7 cm diameter and 14.0 cm length. Detailed description of preparation process can be found in [3,4]. Prepared hydrogen microfoam possesses the following parameters. The foam expansion ratio equals to 10. The average diameter of the bubbles is about 200 µm. Hydrogen-oxygen mixture was prepared using the hydrogen and the oxygen-nitrogen mixture containing 90% of oxygen and 10% of nitrogen. The microphotography of the considered combustible foam is presented in Fig. 1(a) (the general case with heptane addition is shown). The combustion process was analyzed with the use of high-speed video camera Photron FASTCAM SA-4 (100000 fps, 9.5 µs shutter speed).

In this paper, the mathematical modeling of the foam combustion was carried out on the base of the two-phase continuum model presented in [12], with an account of liquid evaporation on the interface between heated gas and liquid phase of the foam according to balance relation presented in [13]. The calculation of the liquid evaporation from the foam surfaces was conducted via tracing the interface and calculating the heat flux from the hot gas to the adjacent foam surface. The foam decay under the action of heat and dynamic effects was modeled via empiric criterion for gas volume fraction \( \alpha_{g} > \alpha_{cr} = 0.96 \). In this way, as soon as the gas volume fraction exceeded a certain critical value the foam decayed into the droplets. The initial diameter of droplets was set to be equal to 140 µm, which corresponded to the average size of Plateau borders in the foam with average bubble diameter of 200 µm. In addition, the Weber criterion was used for the destruction of liquid films between bubbles under the compression. Here, the film was treated as a liquid droplet breaking up by the dynamic pressure of 2 \( 10^6 \) Pa that corresponded to Weber number \( We = 350 \). This value is usually reported as one of the critical points at which the breaking up of the droplets begins [14]. In the gas-droplets region behind the front of foam decay, the heating of the droplets is limited by the processes of phase transformation (evaporation). Here it is assumed that the evaporation of droplets is limited by a heat transfer. Fragmentation of droplets is modeled with the use of Weber criterion. Taking into account the available experimental data on droplets fragmentation [14] one can assess the values both of the induction time \( (\tau_{ind}) \) of the break-up and diameter \( (d) \) of small droplets breaking away from the surface of the liquid droplet. Both values are estimated via empirical dependencies on liquid and vapor properties, dynamic pressure and Reynolds number of the flow [14]. To model hydrogen combustion a well-known contemporary kinetic mechanism from [15] was used.
Figure 1. (a) Microphotography of the foamed emulsion. (b) The structure of the foam model: grey regions contains greater amount of liquid, white regions contains greater amount of gas, grid corresponds to the numerical grid. (c) The geometry of computational domain: grey region – the foam at 300 K temperature, red region – the heated layer \((T = 3000 \text{ K})\). The height of the channel is 14 cm, the width of the channel is 3.7 cm.

An important issue related to the flame propagation in the foam concerns the ratio between the spatial scales determining the flame front and the bubbles. Since the characteristic bubble size is of the order of flame thickness \((L_f \approx 300 \mu\text{m})\), the effect of local interactions between the flame and the elements of liquid phase should be taken into account. In the simplest case such an interaction can be considered as the flame interaction with the grid of liquid droplets of diameter \(~0.7d_b\) spatially separated with grid step \~(1+0.7)d_b\, where \(d_b\) is the bubble diameter and scale \(0.7d_b\) is the characteristic size of the Plateau border. Here it is proposed to utilize continuum representation of two-phase system with imposed initially non-uniform distribution of liquid mass density \(\rho_{\text{liq}}(x, y)\). Herewith, its local maximal values correspond to the centers of Plateau borders, while zero values correspond to the centers of bubbles. The bubbly structure is modeled with the use of sampling algorithm proposed in [16]. The structure of the foam model is presented in Fig. 1(b). According to such problem setup, the corresponding non-uniformity in drag coefficient is introduced that causes the flow perturbations on the scales \~d_b\.

In the experiment, the ignition of the combustible foam was carried out by a pilot flame. To model close conditions of ignition, the foam was ignited by a finite layer of the initially heated gas (Fig. 1(c)). The initial temperature inside the 2 mm layer was 3000 K, and so the ignition arose in the heated zone. Subsequently, the flame was formed at the contact surface between the reacted medium and the adjacent cold layer of the foam.

The calculations were carried out with the use of Euler-Lagrange numerical technique widely used to solve various problems in the field of gaseous and two-phase combustion [17]. The resolution test was carried out. The pre-detonation distance was taken as the test parameter. With the use of traditional Richardson approach [18] it was found that in the range of computational cell sizes from 100 \(\mu\text{m}\) down to 25 \(\mu\text{m}\) the rate of convergence equals to \(k = 1.8\). Herewith, the resolution with 25 \(\mu\text{m}\) cell size provided 0.4% error while the resolution with 100 \(\mu\text{m}\) cell size provided 5.0% error relative the exact solution. Most of the calculations were carried out with the use of computational cells of 50 \(\mu\text{m}\).

3. Results and discussion

Let us consider in details the process of flame propagation through the foam. As one can see (Fig. 2) there are three main stages of flame evolution: flame acceleration, transition to detonation and self-sustained detonation propagation. In particular in the considered case of pure hydrogen-based microfoam (without heptane addition) a monotonic flame acceleration takes place (Fig. 2(a)). Note, that an addition of oil should inhibit hydrogen oxidation kinetics [19], therefore, the reactivity of the combined fuel decreases and non-monotonicity could be observed distinct to the case considered here.
Analysis of the visualization patterns (Fig. 3) shows that the flame evolves in a quite similar manner as in a pure gaseous mixture [20]. On the early stage, the isotropic expansion of the flame out from the ignition source takes place. Further, as soon as the flame surface achieves the side walls, a so-called “finger flame” is formed and propagates along the walls. On this stage local deceleration of the flame can be noticed, however, integrally the flame continues to accelerate. According both to experimental and numerical observations (Fig. 2) flame acceleration can be described with a high accuracy by the exponential law. This indicates that the flame acceleration is defined by the mechanism with positive feedback. When considering the flame propagation in channels [21] or through the porous medium [22, 23], the hydraulic resistance provides such a mechanism. Momentum losses to the walls or obstacles define the flame stretching and its acceleration. Herewith, the larger the flame speed the larger momentum losses are and vice versa. As a result, the exponential acceleration of the flame takes place. In the case of combustible foam, the hydraulic resistance is defined by the interactions between phases like in the porous medium. The main difference is that the foam is unstable and decays under the dynamic action and the heat flux from the flame front. Flame propagation through the foam can be treated as the flame propagation through the “grid” of droplets regularly dispersed in space (Fig. 4(a)). Droplets impact on the flame surface excites short-wave perturbations with a wave-length of the order of bubble size. At the same time, it is known that the flame is intrinsically unstable, and short-wave perturbations grow with the highest rate [24]. Exactly this represents the particular mechanism of flame acceleration in the foam (close pattern was recently observed in [25]). The numerically obtained flame structure is demonstrated in Fig. 4(b). As one can see the proposed model resolves the fine structure of the flame surface excited with short-wave perturbations of the order of bubble size. The proposed model and obtained results provide close quantitative results on the flame speed evolution in the process of flame acceleration (Fig. 2).

The process of flame acceleration is always accompanied by the medium compression ahead of the flame front [26]. Herewith, during the flame propagation through the obstructed channel [10] or porous medium [11] the inner reflections cause energy focusing leading to the local compression up to a quite high rates. In bubbly liquids, the energy focusing can also take place due to the bubbles collapse [5]. In the case of emulsions, the nucleation processes related to the medium superheating can trigger the compression effects [27]. As a result, in all the mentioned cases the compression can lead to the gaseous mixture self-ignition. In such a way, the detonation-like regime driven by the compression-induced ignition can be established. Generally speaking, a similar scenario is realized in the considered case of wet foams bubbled with the combustible mixture. The energy focusing due to the bubbles collapse induces ignition on the scales of the single bubble (Fig. 4(c)). The combustion products expand that leads to the formation of the outwardly propagating compression wave. Such compression waves emitted out from the exploded bubbles induce the collapse and ignition of the neighboring bubbles. That determines the mechanism of reaction wave propagation on the stage following the flame acceleration. The transient stage is characterized by the sharp increase in the flame speed (stage “2” on Fig. 2) that
indicates a drastic change of the mechanism of reaction wave propagation. Hence, the detonation onsets in the foam.

**Figure 3.** Flame evolution in the microfoam bubbled with hydrogen-oxygen mixture, $2\text{H}_2 + \text{O}_2$. Numerals indicate different stages of the process: 1 – flame acceleration, 2 – transition to detonation, 3 – relaxation to the steady-state detonation, 4 – onset of steady-state detonation.

**Figure 4.** (a) Schematic of flame propagation mechanism, F - foam, PZ - preflame zone, CP - combustion products. (b) Numerical resolution of the local structure of the flame front, grey color illustrates the foam structure, temperature field is shown with a color palette. (c) Schematic of the detonation propagation mechanism, IB - initial bubble, S - shock wave, CB - compressed bubble, EB - expanding bubble.

4. Conclusions

In this paper, the main attention is paid to the analysis of different regimes of flame propagation in the microfoams prepared via bubbling of hydrogen-oxygen mixture through the aqueous solution. In particular, the regimes with flame acceleration and subsequent detonation onset are considered in details. In many ways, the flame structure in the considered system is similar to that formed in the porous medium. Permanent excitation of the short wave-lengths on the flame surface favors the instability development that finally determines the exponential acceleration of the flame that represents a peculiar type of hydraulic resistance, which is the leading mechanism of flame acceleration in porous media [22]. The compression waves generated by the accelerated flame compress the medium ahead of the flame front. This leads to the effect of energy focusing (or cumulation) on the scales of individual bubbles in the process of their collapse. As a result, the compression-induced intensification of the reaction takes place, and finally a detonation-like regime of reaction wave propagation through the foam is established.

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