Cavitation-induced ignition of cryogenic hydrogen-oxygen fluids

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The Challenger disaster and purposeful experiments with liquid hydrogen (H2) and oxygen (Ox) tank breaches demonstrated that cryogenic H2/Ox fluids always self-ignite in the process of their sudden mixing. Here, we propose a cavitation-induced self-ignition mechanism that may be realized under these conditions. In one possible scenario, self-ignition is caused by the strong shock waves generated by the collapse of pure Ox vapor bubble near the surface of the Ox liquid that may initiate detonation of the gaseous H2/Ox mixture next to the gas-liquid interface. This effect is further enhanced by H2/Ox combustion inside the collapsing bubble in the presence of admixed H2 gas. [doi:10.1063/1.3571445]

The source for the formation of flames in the cryogenic hydrogen (H2)/oxygen (Ox) fuel mixture during the Challenger disaster in 1986 still remains a mystery. The fireball which caused the orbiter's destruction appeared near the ruptured intertank section between the liquid H2 (LH2) and liquid Ox (LOx) tanks but not near the hot jets from the nozzles.[1,2] Purposeful experiments with Ox and H2 tank breaches carried out by NASA (Ref. 3) showed that cryogenic H2/Ox mixtures always self-ignite when the streams of cryogenic fluids containing gaseous hydrogen (GH2), gaseous oxygen (GOx) and LH2 mix with a turbulent LOx stream. Since this effect can lead to catastrophic evens, understanding its mechanisms is a problem of great importance.

In this letter, we propose a cavitation-induced self-ignition mechanism of cryogenic H2/Ox fluids. Cavitation is the formation and compression of vapor bubbles in liquids under the action of an abrupt pressure jump between the liquid and the gas phases. Due to the inertial motion of the liquid this process leads to a rapid collapse of the bubbles and spiking of the gas temperature and pressure inside, producing strong shock waves.[4,5] Here, we discuss some possible scenarios of cavitation-induced ignition in cryogenic Ox/H2 fluids. We concentrate on the most transparent scenario related to the collapse of a vapor bubble in the Ox liquid near the interface between LOx and the GH2/GOx mixture.

Much like when a bottle of carbonated beverage is suddenly opened, pure Ox vapor bubbles will form in LOx escaping from a ruptured tank as the result of a sudden loss of overpressure. Vapor bubbles with admixed GH2 will also be created in the falling LOx blobs as a result of mixing of GH2 and GOx with a turbulent LOx stream. A pressure jump between LOx and the bubbles may arise, for example, due to shock waves arising as a result of an impact of a LOx blob against a solid object [Fig. 1(a)]. The overpressure in such a shock wave is of order $\Delta p \simeq (1/2)\rho_L v^2 \gtrsim 2$ atm even for moderate velocities $v \gtrsim 20$ m/s of the liquid. Such a "weak" shock wave cannot induce ignition of the GH2/GOx mixture directly, but it can initiate cavitational collapse of the vapor bubbles inside LOx. Our computations presented below show that such weak initiating shock waves can lead to the formation of bubbles of a small radius $R_{\min} \simeq 0.1$ mm with huge pressures $p \gtrsim 1000$ atm and temperatures $T \gtrsim 2500$ K

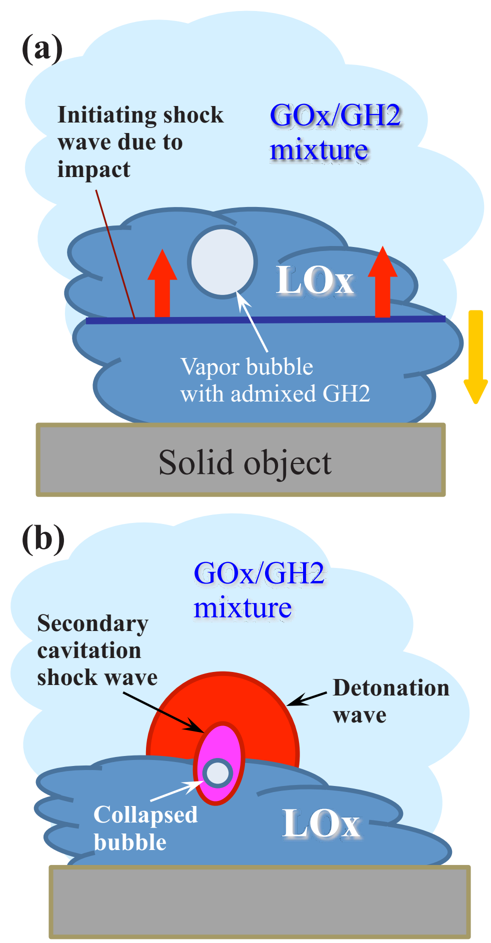

FIG. 1. (Color online) One scenario of cavitation-induced ignition of GOx/GH2 mixture: (a) an initiating "weak" shock wave in a LOx blob (with a bubble) forms due to its impact with a solid object and (b) collapse of the bubble near the liquid-gas interface under the action of the initiating shock wave and generation of a strong secondary shock wave inducing detonation of the GH2/GOx mixture.

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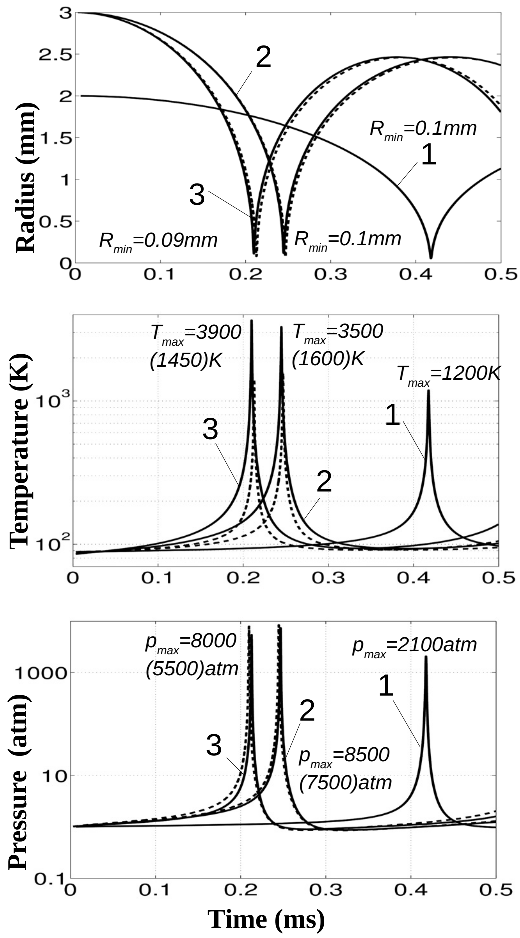

FIG. 2. Bubble collapse dynamics for the initial total gas pressure $p_0 = 1$ atm. Other initial parameters are: radius $R_0 = 2$ mm, overpressure of the initiating shock wave $\Delta p = 0.25$ atm, GH2 partial pressure $p_{H2} = 0$ (curve 1); $R_0 = 3$ mm, $\Delta p = 1.5$ atm, $p_{H2} = 0.01$ atm (curve 2); $R_0 = 3$ mm, $\Delta p = 2.0$ atm, and $p_{H2} = 0.015$ atm (curve 3). The dashed lines and the values in parentheses are obtained without considering combustion in the bubble.

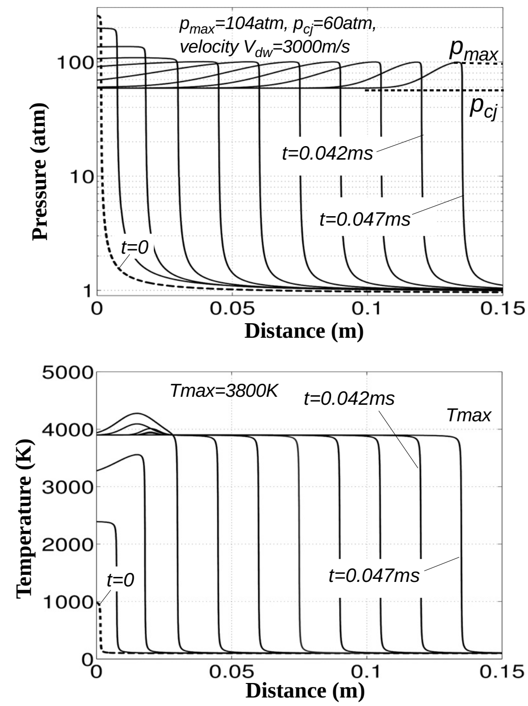

FIG. 3. Formation of cavitation-induced hemispheric detonation wave in stoichiometric H2/Ox mixture with temperature $T = 100$ K and pressure $p = 1$ atm. The initial condition is: temperature $T = 1000$ K and pressure $p = 250$ atm in the central area with radius $r \le 0.15$ mm (dashed curves).

inside (Fig. 2). This causes ignition of the GOx/GH2 mixture inside the bubble. The strong secondary shock wave generated by the cavitational bubble collapse near the LOx interface may then propagate into the gaseous H2/Ox mixture next to the LOx interface [Fig. 1(b)]. We demonstrate that such a localized shock wave is sufficient to induce detonation in cryogenic GH2/GOx mixtures (Fig. 3).

To simulate the bubble collapse, we used the standard fluid dynamics equations describing conservation of the number of particles, energy and momentum under the assumption of spherical symmetry.[4,6] More specifically, we treated the liquid as incompressible and inviscid, neglected surface tension at the interface, treated the gas phase as a mixture of ideal gases and took into account diffusion and thermodiffusion of the admixed GH2 (for more detail see Ref. 7). We also modeled combustion inside the bubble, using a simplified model based on an assumption that the burning rate is limited by the initiation reactions $H_2 + O_2 \rightarrow OH + OH$ and $H_2 + O_2 \rightarrow HO_2 + H$, which have the lowest rates. Thus, we modeled the GH2/GOx combustion by a brutto reaction $H_2 + O_2 \rightarrow H_2O + \frac{1}{2}O_2$ with the rate $G_{comb}(T) = c_{H2}c_{Ox}[1.1 \times 10^8 \exp(-19\,680/T) + 1.48T^{2.433} \exp(-26\,926/T)]$ $m^3/(mol\ s)$, where c_{H2} and c_{Ox} are the molar concentrations of GH2 and GOx, respectively, and T is in degrees kelvin.[8] We note that this approximation is close to the one-step mechanism of Mitani and Williams.[9] Also, the model predicts the same steady detonation wave parameters as those obtained[3] with the help of the model taking into account 17 main chain reactions of GOx/GH2 mixture combustion.[10]

Our simulations show that under the action of an initiating shock wave with overpressure $\Delta p \ge 0.15$ atm the maximum pressure and temperature in pure vapor bubbles of initial radius $R_0 \gtrsim 2$ mm collapsing in LOx exceed 1500 atm and 800 K, respectively, when the bubble radius reaches its minimum value of $R_{min} \simeq 0.1$ mm (curve 1 in Fig. 2). With the increase in Δp the values of p_{max} and T_{max} increase and the value of R_{min} decreases ($R_{min} \le 0.05$ mm at $\Delta p \ge 0.5$ atm). The presence in the bubble of even a small amount of noncondensable GH2 sharply decreases the values of p_{max} and T_{max}. However, at large enough $\Delta p \ge 0.5$ atm and $R_0 \gtrsim 2$ mm the bubble collapse leads to high temperatures and ignition of the Ox/H2 mixture in the bubble. As a result of this local explosion the values of p_{max} and T_{max} in the bubble reach gigantic values $p_{max} \ge 8000$ atm and $T_{max} \ge 3500$ K (Fig. 2). We note that in reality the superhot and supercompressed O, H, and OH species forming in the process of GH2/GOx combustion[10] inside the bubble may be ejected into the space above the LOx surface and easily ignite the GH2/GOx mixture nearby.

The same equations of gas dynamics used in the cavitation simulations were also employed to analyze the ignition of GH2/GOx mixtures by a localized strong shock wave generated by the collapsing bubble. We envision a hemispherical shock wave propagating in the unconfined GH2/GOx mixture above the LOx-gas interface [see Fig. 1(b)], initiated by a local increase in gas pressure and temperature within the radius $R_0 \sim R_{min}$. We see that the local jump of the pressure

$p \gtrsim 200$ atm and temperature $T \gtrsim 500$ K in the GH2/GOx mixture area of radius $R_0 \gtrsim 0.15$ mm is sufficient to induce detonation in stoichiometric GH2/GOx mixtures (Fig. 3).

We now list other possible cavitation-induced scenarios that may lead to self-ignition of cryogenic H2/Ox fluids upon mixing.

(i) Formation of rarefied GOx bubbles in LOx.
(ii) Formation of GOx bubbles in LOx with a thin chilled layer of liquid near the bubble surface.
(iii) Injection of cold LH2 droplets into "hot" LOx.
(iv) Injection of "hot" LOx droplets into cold LH2.

In scenario (i), rarefied bubbles form in the LOx stream impinging on an obstacle and collapse under the liquid pressure. In scenario (ii) bubbles may form as a result of an impact of two large LOx blobs whose surfaces were chilled by contact with very cold ($T \simeq 20$ K) surrounding GH2. Due to the low near-surface temperature the pressure in the bubble may quickly drop because of intense vapor condensation, leading to a rapid bubble collapse. In scenario (iii) the pressure inside the bubble will quickly grow and may become much greater than the pressure p_L in the liquid bulk. As a result, the bubble radius will increase and, due to the inertial motion of the liquid, the pressure in the bubble can become much less than p_L. As a consequence, the bubble will start to collapse, and the gas temperature and pressure inside the bubble may achieve very high values, initiating a local explosion and a strong shock wave. Finally, in scenario (iv) heavy droplets of LOx may penetrate deeply into LH2 (a light fluid), causing intense evaporation of LH2 and formation of a GH2/GOx bubble inside LH2 that will grow in size and then collapse due to inertial motion of the liquid. Since the critical temperature $T_c = 33.2$ K of H2 is significantly below the freezing temperature $T_m \simeq 54$ K of LOx, the evaporation of LH2 in contact with LOx may acquire an explosive character, resulting in even more dramatic outcomes. We note that in addition to these scenarios occurring at the liquid/gas interface, more complicated scenarios involving creation of cavitating bubbles in the turbulent LOx stream in the vicinity of ruptured tank walls are also conceivable.

To summarize, we have identified a possible mechanism of ignition in cryogenic H2/Ox fluids which relies on the generation of strong shock waves by the cavitational collapse of vapor bubbles close to the liquid-gas interface in the process of cryogenic H2/Ox mixing. While only one such bubble is sufficient to ignite the adjacent GH2/GOx mixture, the presence of many bubbles will make the occurrence of the right conditions for our mechanism to work much more likely. We showed that the presence of LOx blobs surrounded by GH2/GOx mixture may be sufficient to initiate H2/Ox ignition, including strong detonation waves. We further proposed several other scenarios that include mixing of LH2 with LOx and resulting in even more dramatic consequences. More detailed studies of these mechanisms are currently underway. Finally, we note that the obtained insights into the self-ignition mechanisms should be very important for understanding conditions and risks of explosion in cryogenic H2/Ox-based liquid rockets and other space vehicles.

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