ARTICLE NO. 80-4099

J80-234

Evolution of a Detonation Wave in a Cloud of Fuel Droplets: Part II. Influence of Fuel Droplets

20015
60003

Alexander Burcat* and Shmuel Eidelman†
Technion—Israel Institute of Technology, Haifa, Israel

This is the second part of an investigation in which the whole problem of energy release in a combustible spray-gas mixture is solved. The influence of the droplet size of the spray on the parameters of the shock waves traveling in the media are delineated. The investigation was able to reveal the mechanism of shock wave reinforcement and to show the source of dynamic instabilities encountered with two-phase detonation processes.

Nomenclature

D = detonation wave velocity
E_0 = energy of the igniting source
ℓ = average radius of the droplet
L = heat of evaporation
n = normalized number of drops per unit volume
P = pressure
Q = thermal effect of the chemical reaction per unit mass of fuel
r_0 = initial radius of the igniting source
r = space variable
t = time
T = temperature
V = mass velocity
γ = effective isentropic exponent of the gas
λ = the undimensional size of a drop
μ = dynamic viscosity
ρ = average density of the component
κ = heat conduction coefficient of the gas

Superscripts and Subscripts

i = initial value
sa = shock average

I. Introduction

IN Part I of this paper,[1] the influence of an igniting explosion source was investigated with the purpose of igniting and detonating a fuel spray dispersed in an oxidizing atmosphere.

The influence of the energy density and the energy quantity of the igniting explosion was well delineated in a series of computations taking into account the chemico-physical parameters of the two-phase media.

In Part II of the research, it is intended to describe the influence of droplet size and its motion on the detonation parameters of the cloud, to study in depth the reinforcement mechanism of the shock wave by the energy liberated in the cloud, and to study the effects of droplet size on the blast wave behind a cloud of a finite size.

Received Oct. 3, 1979; revision received Feb. 25, 1980.

Index categories: Combustion Stability, Ignition and Detonation; Shock Waves and Detonations.

*Senior Lecturer, Dept. of Aeronautical Engineering.

†Instructor, Dept. of Aeronautical Engineering.

II. Exposition and Computations

In Part I of this study, a general and detailed exposition of the problem was presented including the mathematical model and the basic assumptions. Details of the solution and the algorithm for calculations were presented elsewhere.[2] For details, Part I of this publication should be consulted.

III. Results

A. Influence of the Energy Source on Droplet Behavior

In this study, the influence of droplets on the detonation of a fuel cloud dispersed in an oxidizing gas has been investigated. As in Part I, the dispersed liquid is heptane in oxygen. The parameters used for the first experiments (the ones already discussed in Part I[1]) are $\ell_i = 10^{-4}$ m; $L = 3.6 \times 10^5$ J/kg; $\rho_2^i = 675$ kg/m^3; $\mu_2 = 3.7 \times 10^{-4}$ kg/s·m; the boiling point of heptane is 330 K.

For the oxygen, $\rho_1^i = 1.3$ kg/m^3; $\mu_1 = 0.207 \times 10^{-4}$ kg/s·m; and $\kappa = 0.1$ W/m°C. The oxygen fuel ratios were all stoichiometric and for these conditions $\gamma = 1.17$ and $Q = 40 \times 10^6$ J/kg (fuel) were calculated with the Gordon and McBride program.[9]

Figure 1 represents the graphs for the velocity of a drop V_2, the undimensional size of a drop λ, and the number of drops per unit volume n.

The parameters for an igniting explosion are $E_0 = 1.25 \times 10^6$ J, $r_0 = 0.1$ m, along with the rest of the parameters as previously described. These are the same conditions as for Fig. 2 in Part I of this study. The graphs are represented in similar time steps. There, the blast wave decays faster than in the first case, and therefore, the droplets shatter at a longer distance causing a "plateau" of unchanging parameters at a distance of 0.025 m behind the shock front. When the shock gets reinforced, the droplets get shattered faster and so, the plateau diminishes.

Therefore, it can be summarized that when the igniting energy is big enough to cause direct transition to detonation, the droplets are shattered almost immediately behind the blast front. When the energy is smaller and the blast front velocity first decays before being reinforced, and then achieves the detonation velocity, the droplets attain a constant velocity behind the shock front during the blast's decay, and the rate of their disintegration increases only when the blast wave's velocity increases.

B. Influence of Droplet Size on Detonation of the Media

The shattering rate of droplets depends on the droplets' size. On the other hand, the droplets' shattering determines the rate of release of the chemical energy behind the blast wave. Therefore, the droplets' size must have a big influence on the detonation parameters of the media.

The following parameters for the igniting explosion were chosen—$E_0 = 1.25\times10^6$ J and $r_0 = 0.1$ m—for the purposes of studying how droplet size influences detonation parameters.

The fuel was heptane C_7H_{16} with the parameters $L = 3.6\times10^5$ J/kg; $\rho_2^i = 675$ kg/m³, $\mu_2 = 3.7\times10^{-4}$ kg/s·m; and the boiling point is 330 K. Pure oxygen was the oxidizing medium where $\rho_l^i = 1.3$ kg/m³; $\mu_l = 0.207\times10^{-4}$ kg/s·m; and $\kappa = 0.1$ W/m°C. These parameters remained unchanged for all the calculations in this set. However, the size of the droplet radius (ℓ^i) was varied between 5×10^{-5} and 5×10^{-4} m.

Figure 2 represents the pressure velocity and density of the shock wave for droplets of the radius of 50 μm ($\ell^i = 5\times10^{-5}$ m). As pointed out by Nicholls et al.,[4] the parameters of the blast wave in a media with droplets of this size or smaller behave like in a perfect gas, and the influence of the two-phase medium is not observed.

The detonation parameters obtained are $\rho = 5.5$ kg/m³; $P = 72\times10^5$ N/m²; and $D = 2375$ m/s. For reference, the detonation velocity of gaseous heptane and oxygen is $D \cong 2400$ m/s.

In Figs. 3 and 4, the influence of the droplet size on the pressure and velocity of the wave's front is shown. Graphs 1-5 in the two figures differ from each other by the size of the droplets only. The velocity increases 2.3 times when the droplet diminishes in radius from 500-50 μm. The parameters for graph 1 (where $\ell^i = 50$ μm) are almost equal to the parameters of detonation in gases.

The fluctuation of pressure for graphs 3 and 5 in Fig. 4 are caused by the appearance of secondary shock waves (see Sec. C).

Figure 5 represents the graphs of shock speed and the width of the reaction zone as a function of droplet size. The scale of the reaction width zone was arranged so that its zero coincides with the zone in a phase where heptane droplets of 500 μm coincide with the detonation velocity in this mixture. The figure presents good agreement between both curves, which shows an inverse relationship between the detonation velocity and the width of the reaction zone. It can be seen that the dependence between the detonation velocity and the particle size is parabolic.

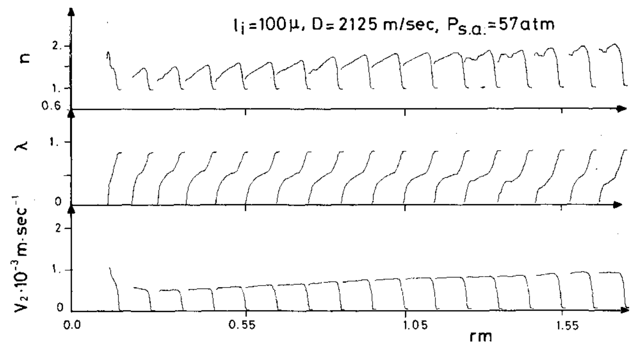

Fig. 1 Velocity, undimensional radius λ, and the number of drops per unit volume for the liquid phase vs the radius of the shock; $E_0 = 1.25\times10^6$ J, $r_0 = 0.1$ m.

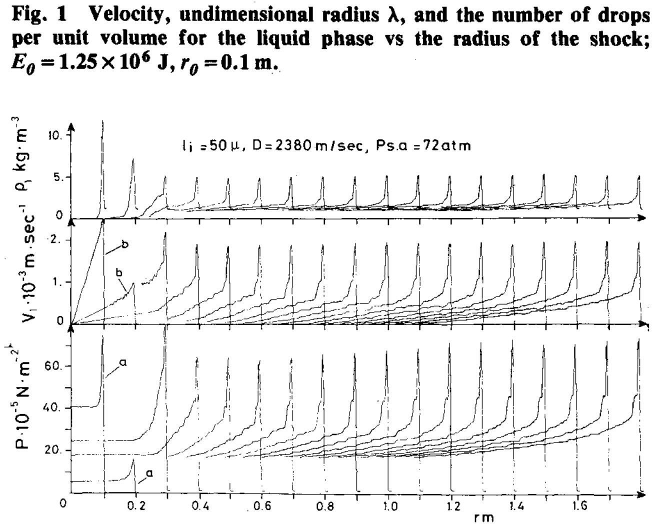

Fig. 2 Pressure, velocity, and density of the gas phase vs the radius of the shock: $E_0 = 1.25\times10^5$ J; $r_0 = 0.1$ m; and $\ell^i = 5\times10^{-5}$ m. a) $P\times10^{-6}$ N/m²; b) $V\times3.29\times10^{-3}$ m/s.

C. Mechanisms of Reinforcement of the Blast Wave in a Two-Phase Medium

When a very dense computational net was used or in cases where the width of the reaction zone was large, it was possible to follow up the mechanism of reinforcement of the blast wave.

Figure 6 represents computations for an explosion energy equal to $E_0 = 1.25\times10^6$ J and $r_0 = 0.1$ m. The size of the droplets is $\ell_i = 1.5\times10^{-4}$ m, and the computation was performed with a calculating net of $\Delta h = 0.0025$ m.

Secondary waves appear behind the principal shock front at radii of 1 m and up. The local secondary wave appear at some distance, e.g., 0.8 m for the pressure, and travel forward through the reaction zone getting closer and closer to the main wave, increasing in time and finally coinciding with the main wave, thus reinforcing it.

The reinforced front of the shock encounters now higher counterpressure from the undisturbed medium; therefore, it starts to decay until the wave is reinforced again by another secondary wave.

The local reinforcement of the shock wave causes a shortening of the reaction width, in turn causing the increase in the shock's speed.

The secondary wave's length and amplitude are dependent on droplet size, as can be seen in Fig. 7, which was calculated with droplets having a radius of 300 μm. Here, the secondary wave is wider and its velocity relative to the shock front is smaller.

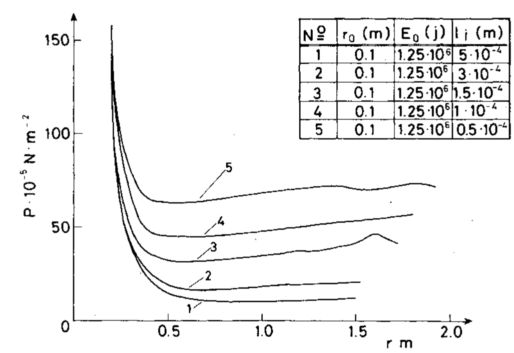

Fig. 3 Pressure on the shock front vs the radius of the shock as a function of droplet size.

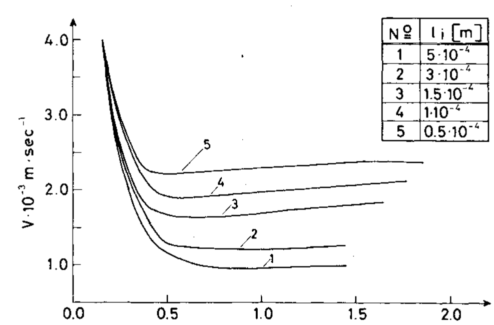

Fig. 4 Shock front velocity vs radius of the shock as a function of droplet size.

Finally, the experimental follow-up after the reinforcement phenomenon leads to the conclusion that the detonation wave is unstable and, thus, the secondary waves or the ripple in the main shock front were called "instabilities."[3-5]

A more detailed study on this problem is presented elsewhere.[10]

D. Influence of the Detonation Outside the Fuel Cloud

The influence of the detonation and the fuel droplets in cases where the cloud is determined in size and the area of interest is beyond the cloud's boundary was also calculated.

Figure 8 represents the pressure behavior in two cases with a cloud whose size is $r = 1$ m. In case 1 the droplet's radius is 200 μm and in case 2 the droplet's radius is 50 μm (i.e., equivalent to a pure gaseous mixture). As can be seen at the boundary of the cloud, the pressure of two different cases drops to the same pressure within the first 20 cm outside the cloud, since the amount of energy liberated in each cloud is equal.

IV. Discussion

The size of the droplets was found to be of crucial importance to its influence on the detonation parameters. It was found that in the range of 50-500-μm radius, the detonation velocity is inversely proportional to the width of the reaction zone behind the shock front. The detonation velocity attained with $\ell^i = 50$ μm is almost equal to the detonation velocity in gases; therefore, further decrease of the droplet size will not cause any increase in the detonation velocity.

In this investigation, it was possible to study some parameters in further detail by increasing the density of the numerical grid.

It was found that in cases where the region of droplet shattering was wide, a plateau of constant gas-dynamic parameters appeared at some distance behind the shock front. The "plateau" length is equal to the width of the shattering region.

It was stated in a few investigations that the propagation of a detonation wave in a two-phase media is accompanied with instabilities.[3-6]

Some models for the reinforcement of the shock wave[7,8] explain the instabilities by discrete release of energy.

In the computations presented here, it was shown that secondary shocks appearing in the reaction zone cause the strengthening of the shock wave. The reinforcement process has a time rate cycle which is explained by the fact that each secondary wave needs approximately the same time in order to reach the main shock wave.

From Figs. 5-7 it can be concluded that the main reason for the diminishment of the detonation velocity with the increase of droplet size is the increasing of the shock front width. This is a different and better explanation than the one forwarded by Cherepanov,[7] who assumed energy losses because of discrete internal explosions.

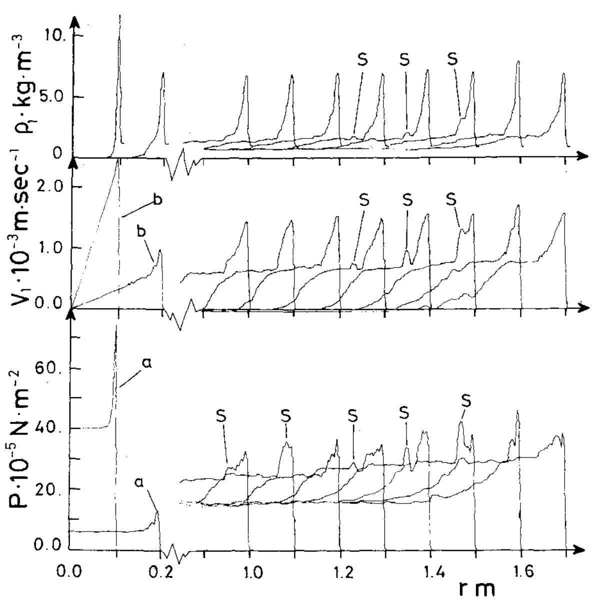

Fig. 5 Comparison of the shock speed vs the droplet size with the width of the reaction zone vs droplet size.

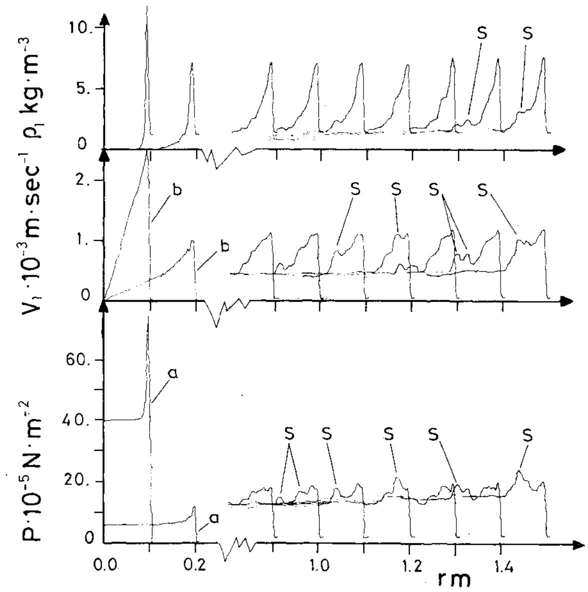

Fig. 6 The pressure velocity and density of the gas vs the shock radius for droplets with a radius of 150 μm and calculated on a dense net $\Delta h = 0.0025$; $D = 1800$ m/s; $P_{sa} = 40$ atm. a) $P \times 10^{-6}$ N/m^2; b) $V \times 3.29 \times 10^{-3}$ m s^{-1}; S = secondary waves.

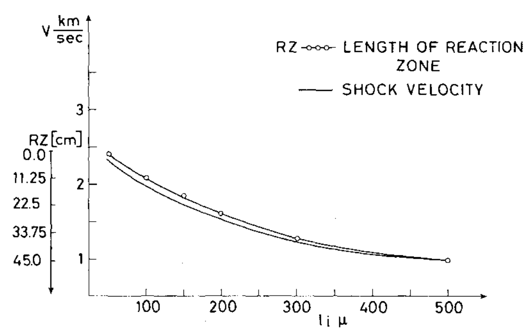

Fig. 7 The pressure velocity and density of the two-phase medium vs the shock radius for droplets with a radius of 300 μm and calculated on a grid $\Delta h = 0.0025$ m: $D = 1250$ m/s; $P_{sa} = 18$ atm. a) $P \times 10^{-6}$ n/m^2; b) $V \times 3.29 \times 10^{-3}$ ms^{-1}; S = secondary wave.

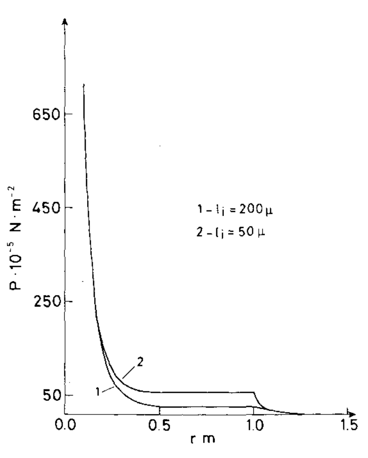

Fig. 8 The pressure developed as a function of the shock radius within and outside the cloud boundaries. The size of the cloud is 1.0 m.

Summarizing, this investigation has shown in detail the influence of the droplets' size on the detonation parameters both in finite cloud and within an infinite cloud. It has also shown that the instabilities encountered in the media are caused by secondary shocks emitted by the reacting media which also travel forward to reinforce the main front. Thus, the mechanism of shock reinforcement was also successfully explained.

References

[1]Eidelman, S. and Burcat, A., "The Evolution of a Detonation Wave in a Cloud of Fuel Droplets: Part I. The Influence of the Igniting Explosion," *AIAA Journal,* Vol. 18, Sept. 1980, pp. 1103-1110.

[2]Eidelman, S. and Burcat, A., "Numerical Solution of Nonsteady Blast Wave Propagation in Two-Phase ("Separated Flow") Reactive Medium," Technion-Aeronautical Rept. 388, Israel, 1980; to be published in *Journal of Computational Physics.*

[3]Pierce, T. H. and Nicholls, J. A., "Time Variation of the Reaction Zone Structure of Two-Phase Spray Detonations," *14th Symposium on Combustion,* The Combustion Institute, Pittsburgh,, Pa., 1973, p.1277.

[4]Nicholls, J. A., Sichel, M., Fry, R., and Glass, D. R., "Theoretical and Experimental Study of Cylindrical Shock and Heterogeneous Detonation Waves," *Acta Astronautica,* Vol. 1, 1974, p. 385.

[5]Gabrijel, Z. and Nicholls, J. A., "Cylindrical heterogeneous Detonation Waves," *Acta Astronautica,* Vol. 5, 1978, p. 1051.

[6]Dabora, E. K. and Weinberger, L. P., "Present Status of Detonations in Two-Phase Systems," *Acta Astronautica,* Vol. 1, 1974, p. 361.

[7]Cherepanov, G. P., "The Theory of Detonation in Heterogeneous Systems," *Prik. Mech. Tech. Fiz.,* No. 4, 1965, p. 163.

[8]Dabora, E. K., "A Model for Spray Detonation," *Acta Astronautica,* Vol. 6, 1979, p. 269.

[9]Gordon, S. and McBride, B. J., "Computer Program for the Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations," NASA SP-273, 1971.

[10]Eidelman, S. and Burcat, A., "The Mechanism of Detonation Wave Enhancement in a Two-Phase Combustible Medium," Technion-Aeronautical Rept. 393, Israel, Jan. 1980.