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Transactions on Aerospace Research eISSN 2545-2835, VOL. 267, NO. 2/2022, 1-12
DOI: 10.2478/tar-2022-0007

THE CONTRIBUTION OF A. K. OPPENHEIM TO EXPLAINING THE NATURE OF THE INITIATION OF GASEOUS DETONATION IN TUBES

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Abstract

This paper analyzes A.K. Oppenheim's original works on the transition of deflagration to detonation and reviews them from the perspective of new numerical and experimental results recently obtained on such phenomena. Particular attention is focused on processes happening in the boundary layer of the tube walls ahead of the accelerating flame. The results of the theoretical analyses of temperature variations inside developing boundary layer are presented and compared to the temperature variation in a free stream away from the boundary layer. Analyses of temperature increase in such layers clearly indicate that the self-ignition of the mixture happens in the boundary layer ahead of the propagating flame front. New experimental results obtained recently by a research group from the A. V. Luikov Heat and Mass Transfer Institute in Minsk, Belarus, combined with previously conducted theoretical analyses and numerical simulations, show clearly and unambiguously that the origin of the "explosion in the explosion", postulated by A. K. Oppenheim in 1966, is always responsible for the Deflagration-Detonation Transition (DDT) in gases and is located in the boundary layer ahead of the accelerating flame front.

Keywords: boundary layer, ignition detonation initiation, combustion, explosion in the explosion, detonation, deflagration-detonation transition (DDT).
Type of the work: research article

1. INTRODUCTION

There are two possible ways to initiate gaseous detonation in tubes: (i) direct initiation by a strong energy source and (ii) ignition of a combustible mixture by relatively weak energy source and then flame acceleration resulting in a deflagration to detonation transition, or DDT. It is also possible to shorten the transition distance or speed up the DDT by inserting some elements in the tube which will increase flame propagation velocity by generating turbulence. The most popular method for this purpose is the "Schelkin spiral" [1], obstacles [2] or even the addition to the mixture of large insert particles [3–5]. For direct initiation of detonation in tubes, energy higher than the critical is required. Such detonations can usually be initiated by a strong shock wave created by an auxiliary shock/detonation tube, condensed explosion, or very strong laser or electrical spark. If the energy is not sufficient, only a shock wave is generated, followed by deflagration. In such cases in relatively long tubes, the flame can accelerate and eventually transition to detonation will occur. This paper discusses

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ARTICLE HISTORY **Received** 2021-11-22 **Revised** 2022-02-02 **Accepted** 2022-04-04

only the problems associated with a relatively weak ignition source and the process of self-acceleration resulting in the abrupt onset of the detonation, based on already published papers, as well as a new finding based on recent experimental work conducted by a group of scientists from the A.V. Luikov Heat and Mass Transfer Institute in Minsk. Taking into account all those findings, final explanations for the mechanism leading to DDT are given.

2. EARLY RESEARCH ON DDT

Initial experimental research on DDT in gaseous mixtures was initiated in the last century in Novosibirsk. In 1959, Salamandra et al. first obtained detailed pictures showing all stages of flame acceleration and transition into detonation [6]. Also, Babkin and Kozachenko [7] and Soloukhin [8] conducted experimental visualizations of such processes. Much research on this subject was conducted from that time and detailed descriptions of these processes can be found in [9]. Most of this research was focused on DDT studies in very reactive mixtures, usually in rectangular tubes. This configuration of the experiments allows one to use optical visualization methods for the processes studied, but direct streak pictures were also recorded to monitor the transition to detonation. One of the first pictures of such a process, obtained by Soloukhin, is presented in Fig. 1 [8].

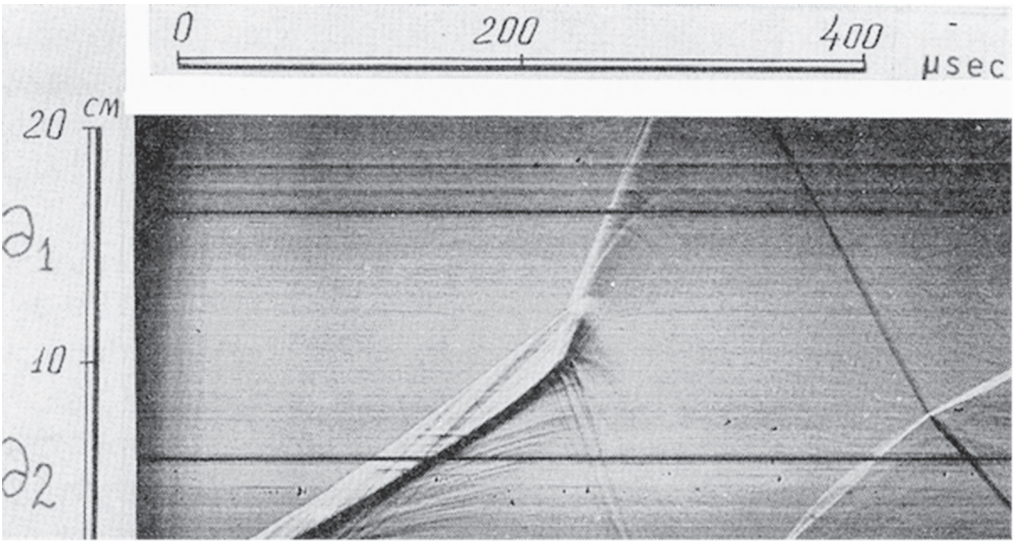


Fig. 1. Streak Schlieren picture of flame acceleration and transition to detonation in an oxy-acetylene mixture in a rectangular tube [8].

In this figure one can clearly see the region of the origin of detonation, as well as two retonation waves propagating in opposite directions, mostly in the combustion products. From such early experiments, the process of transition to detonation was described as follows: in a tube, after ignition of the mixture by a weak energy source, the flame accelerates initially due to the expansion of hot combustion products and generates pressure waves. Behind the pressure waves and just ahead of the flame front, a flow is induced in the unburned combustible mixture. This flow increases the turbulence level of the unburned mixture ahead of the flame front and thus intensifies turbulence combustion, thus the flame propagation velocity is continuously increasing. The accelerating flame generates additional, more intense pressure waves, which support and intensify the leading shock wave and the turbulence generated, so there is strong feedback between the accelerating flame, pressure waves, and shock wave

generation, and the intensity of turbulence combustion. At a sudden point, flame acceleration is sufficient to generate the DDT. During DDT, a local explosion creates very high pressures, and in the transition region, the velocity of the detonation front is usually stronger than its theoretical value (i.e., an overdriven detonation). This is because during acceleration, pressure between the ignition point and the shock front is always increased, and when the transition happens in higher pressure, then the velocity and pressure are higher than calculated for the initial stage. It is also higher than in the still quiescent mixture just ahead of the front shock wave, so when the detonation front enters the quiescent mixture before the leading flame front, the detonation velocity as well as the pressure ratio will approach the C-J condition.

Two basic interpretations of this process have been proposed. One, associated with the A. K. Oppenheim school, called this the self-accelerating process which triggers detonation: the "explosion in the explosion", while the other is linked to the Zeldovich gradient "spontaneous combustion" mechanism.

3. A.K. OPPENHEIM'S RESEARCH ON THE DDT

A. K. Oppenheim was mostly involved in gaseous detonation research starting in 1960 and continuing to 1970, but the most valuable results were obtained in the mid-sixties when he was deeply involved in DDT research as well as detonation structure using a specially developed high speed Schlieren stroboscope system with the laser light source controlled by a Kerr Cell. This technology allows very high time and spatial resolution pictures of the process of the flame acceleration and the DDT in the hydrogen-oxygen mixtures to be obtained. Oppenheim, with his PhD students, conducted pioneering experimental research and theoretical analyses of the DDT and other aspects of detonation as well as dynamic processes associated with the shock waves propagating in combustible mixtures. All pictures from that time were taken in a rectangular channel of cross-section 1×0.5 inch and about 1 m long. More details on this system can be found in [10]. A few pictures from the many obtained during this research, which illustrate DDT in the hydrogen-oxygen mixtures, are presented below. As indicated in Fig. 2 there were four different typical locations of the DDT, but most frequently it was located between the flame front and the leading shock wave. Also, sometimes the location of the DDT was linked to the flame front position, at the contact discontinuity, as well as on the front of the shock wave generated by the accelerating flame. More such pictures showing different stages of the DDT obtained by A.K. Oppenheim and his PhD students can be found in his publications [10–14].

All pictures are actually 2-D images, since the Schlieren integrates all features from the 0.5 inch channel width to the plane (2-D) picture, and since flame propagation in the channel usually has a tulip like (or cone) shape, so there are most often difficulties to guess, or define, the real position of the DDT as related to the flame position, and the exact interpretation of DDT position relative to the flame front is not possible in some cases. In fact, the exact explanation of the nature of origin of the DDT, which in reality occurs ahead of the flame front, was difficult to explain at that time, and a more precise explanation of the nature of such behavior had to wait for further development in the numerical analyses of such processes. This was, however, discussed by AKO in one of his papers with Meyer and Urtiew, in which they analyzed the difficulties of explaining the processes triggering DDT, using the classical gasdynamic boundary layer approach [14]. It should be noticed that in all DDT cases presented by the AKO team, the origin of the DDT center was always located either on the bottom or top of the detonation channel. DDT was never observed at the center of the tube. One reason for this was that both walls were actually very smooth glass windows which did not support the development of an intense turbulent boundary layer. Thus, since the DDT usually happened at the bottom or top surface of the channel, it can also be anticipated that the most favorable regions for development of a strong turbulent boundary layer will be in the corners, between the bottom/top surface of the tube and the window walls.

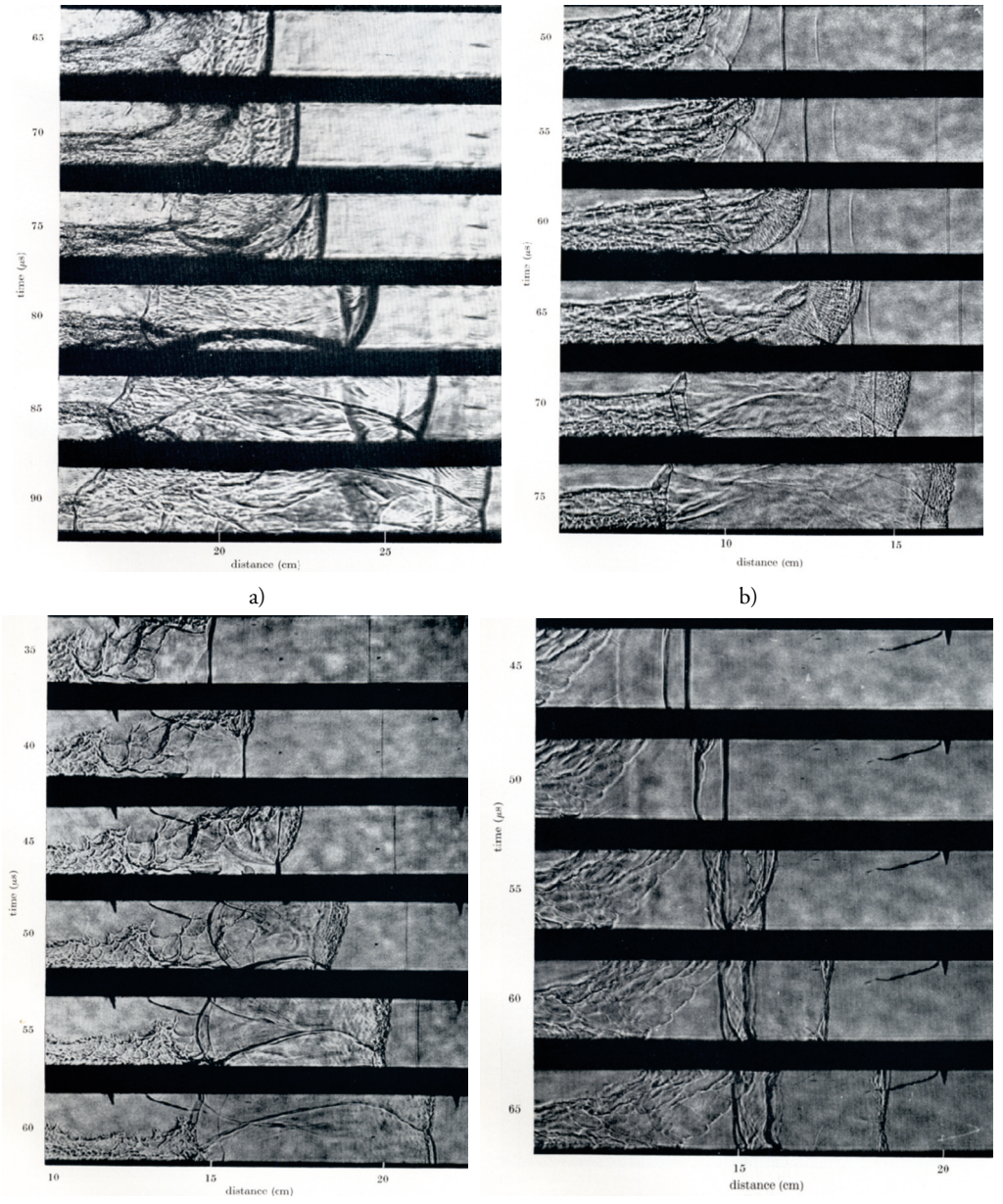


Fig. 2. High-speed Schlieren stroboscopic pictures showing the transition from deflagration to detonation in a hydrogen-oxygen mixture: (a) DDT between the flame and the shock, (b) DDT at the flame front, (c) DDT at a shock front, (d) DDT at the contact discontinuity [12].

Additionally, connections between windows and both bottom/top surfaces of the detonation tube were most probably not perfectly smooth, so the corners of the rectangular detonation tube were the best places for development of the more intensive turbulent boundary layer. In such a "corner" boundary layer, temperature increases due to interference between the induced supersonic flow and the two walls, perpendicularly oriented to each other; this will generate a higher temperature rise by the non-isentropic

process of friction. Consideration of the effect of the boundary layer originated in the corner of this rectangular tube should be sufficient to explain all the DDT cases observed. It was already shown that, by taking into consideration the maximum temperature in such a boundary layer, ignition can be as much as 25 times shorter than for the particle in a free stream beyond the shock wave [15]. It is naturally the case that the application of recent numerical tools could be even more helpful in definitively explaining all aspects of the DDT in tubes.

4. INFLUENCE OF NON-ISENTROPIC PROCESSES ON DDT

The influence of the non-isentropic processes on flame acceleration and DDT was initially identified in the correlations with the studies of flame acceleration and DDT in gaseous mixtures in the presence of large inert particles (sand or silicon carbide), initially at the Warsaw University of Technology [3-4], and later at the Department of Aerospace at the University of Michigan [5]. It was found that the addition of relatively large inert particles can not only accelerate the DDT but can also extend detonability limits. The main reason for this was the generation of micro turbulence, even before ignition; the interaction of large particles dropping in a tube filled with the detonable gaseous mixture. However, after igniting the combustible mixture, the expanding flame generates a flow ahead of the flame which further intensifies mixture flow around the large inert particles and generates even more intense turbulence. When the generated flow becomes supersonic, bow shocks are formed around particles (Fig. 3); also, local hot spots are formed at the front of each large inert particle, still mowing slowly compared to the velocity of the gaseous mixture. This results in an increase in the local temperature and facilitates the process of local ignition. It was already postulated that highly non-isentropic processes occur when large particles interact with supersonic flow and such interactions resulted in significant temperature increase [16]. This also indicated the influence of non-isentropic processes on temperature increase in the turbulent boundary layer generated by the accelerating flame in the tubes/channels, which lead to detonation transition [15]. Thus, at very high concentrations of large particles in the combustible mixture, local ignitions could be facilitated in many locations so that the transition to detonation occurs in smoothly, and only very weak evidence of DDT is observed. This is clearly seen in Fig. 4, where only in Fig. 4a is the transition to detonation seen with a visible abrupt change in the propagation velocity and after this the propagation velocity of detonation remains constant. For the two other cases, Fig. 4 b and Fig. 4c, transition to detonation (constant propagation with velocity close to the theoretical) occurs without clearly visible sharp/abrupt velocity increases (characteristic of DDT in gaseous mixtures) and only very weak, barely visible retonation waves propagated in the post-flame region, as shown in the figures. These waves might also be incident-shock generated at the early stage of flame acceleration and reflected from the end of the detonation tube.

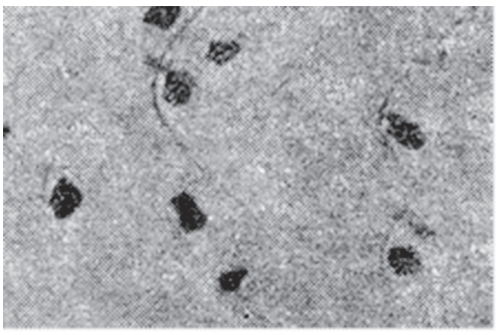
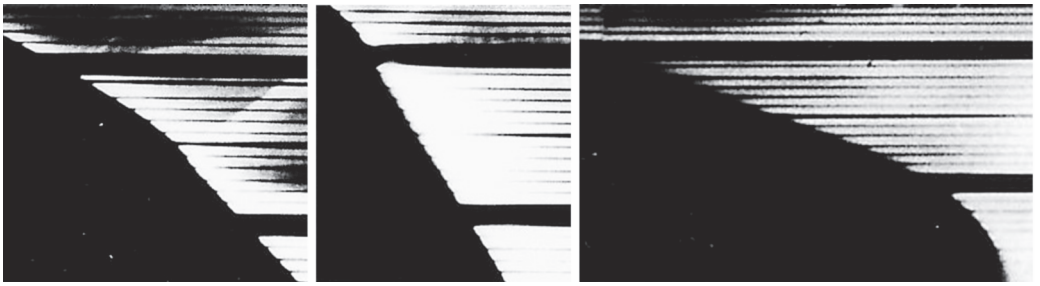


Fig. 3. Interaction of large silicon carbide particles with the supersonic flow of combustible mixture in the tube. The 5% methane-air mixture, gas flow velocity ~1400 m/s, silicon carbide particle average diameter of 1,035 mm [5].

Later detailed analysis of such processes was conducted for the case of flame acceleration in the tube without particles, and strong evidence of significant temperature increase in the boundary layers was observed [17-18]. In Fig. 5, temperature variations in different locations in the turbulent boundary layer show that close to the tube wall, the temperature in the boundary layer is higher and calculations show a significant decrease in the induction time of the gaseous mixture as compared to a free stream particle located at the center of the tube. The mixture parameters and all assumptions are described in [17–18].



a) b) c)

Fig. 4. Direct streak photography of flame acceleration into detonation in gaseous mixtures with the presence of large inert particles: a) stoichiometric hydrogen-air mixture, sand particle concentration 2.14 kg/m^3, b) stoichiometric hydrogen-air mixture, sand particles concentration 3.57 kg/m^3, c) stoichiometric propane-butane-30% oxygen enriched air, sand particles concentration 0.79 kg/m^3 [3].

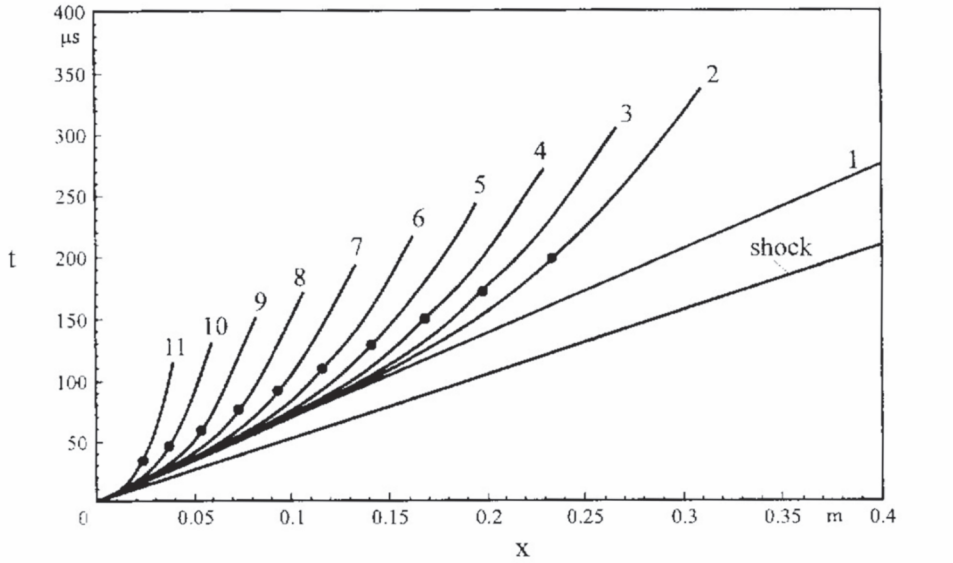
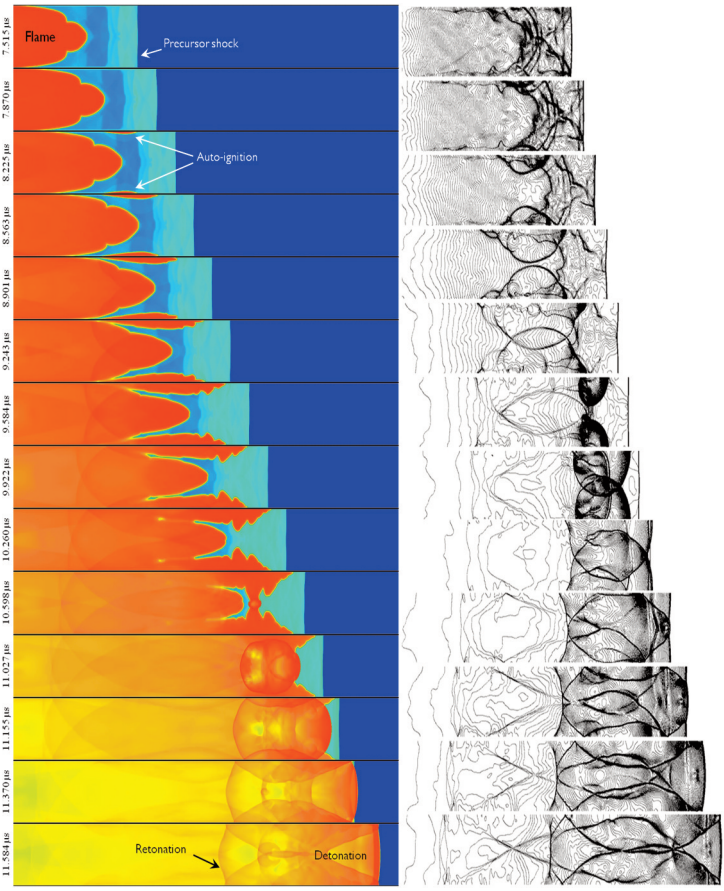


Fig. 5. The predicted time-distance diagram for 11 fluid particles moving behind a shock wave of M=3.5. Particle 1 represents free stream conditions, while particles 2–11 are in the boundary layer at different distances from the wall. The dark cycle shows the time and position of particle ignition. The ignition time of particle 1 is much longer and is located outside the plot [17].

The friction between the moving mixture and the wall is the source of a temperature rise ahead of the flame front. It was shown for the first time that these highly non-isentropic processes which occur in the boundary layer generate a sufficient local temperature increase to trigger the ignition and explosion of the mixture in the boundary layer [17–18]. Later 2-D numerical simulations, performed by

E. Dzimińska et al. [19] clearly showed development of the ignition in the boundary layer which later develops into a local explosion, initiating a local shock which triggers DDT. This process is clearly visible in the numerically obtained temperature and pressure field for flame acceleration in tube and is presented in Fig. 6 a, b [19].



a) b)

Fig. 6. Numerical simulation of DDT in a hydrogen-oxygen mixture triggered by non-isentropic processes in boundary layer, temperature (a) and pressure (b) contours. (courtesy of A.K. Hayashi et al.)[19].

Even more detailed numerical simulations of DDT were performed by Matchida et al. [20]. They clearly show that the ignition happened in tube corners where adiabatic processes, which happen in the boundary layer, are essential for triggering the DDT ahead of the flame front (Fig. 7). They also performed detailed simulation of one famous A.K. Oppenheim picture showing the initiation of detonation in a hydrogen-oxygen mixture (Fig. 8). It can clearly be seen that they were able to create an exact simulation of the DDT, and show that processes happening in the boundary layer in tube corners are responsible for the transition.

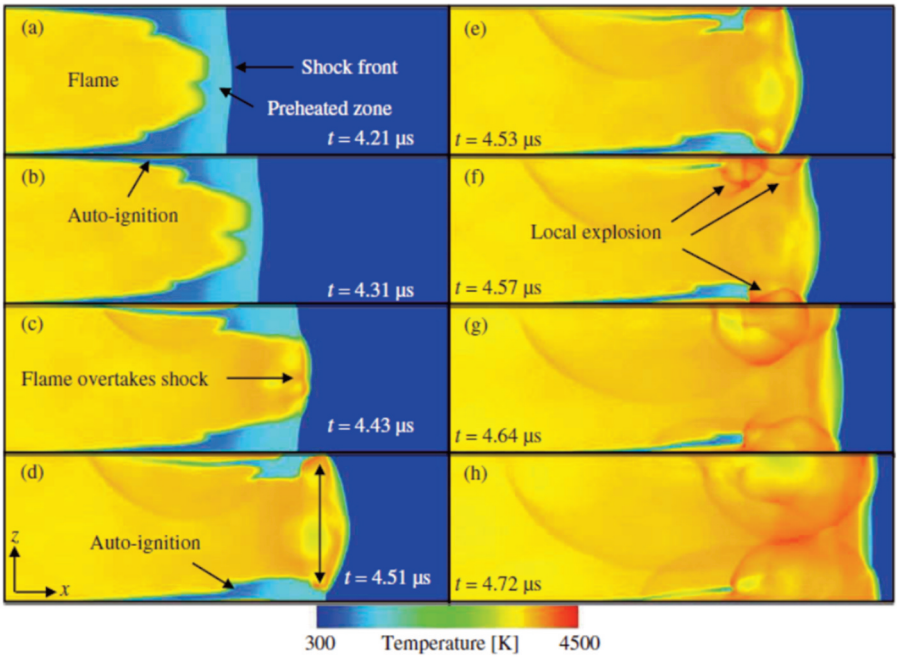


Fig. 7. Detailed DDT process in the adiabatic case shown on x-z plane at the center of the y-direction (courtesy of Machida et al. [20]).

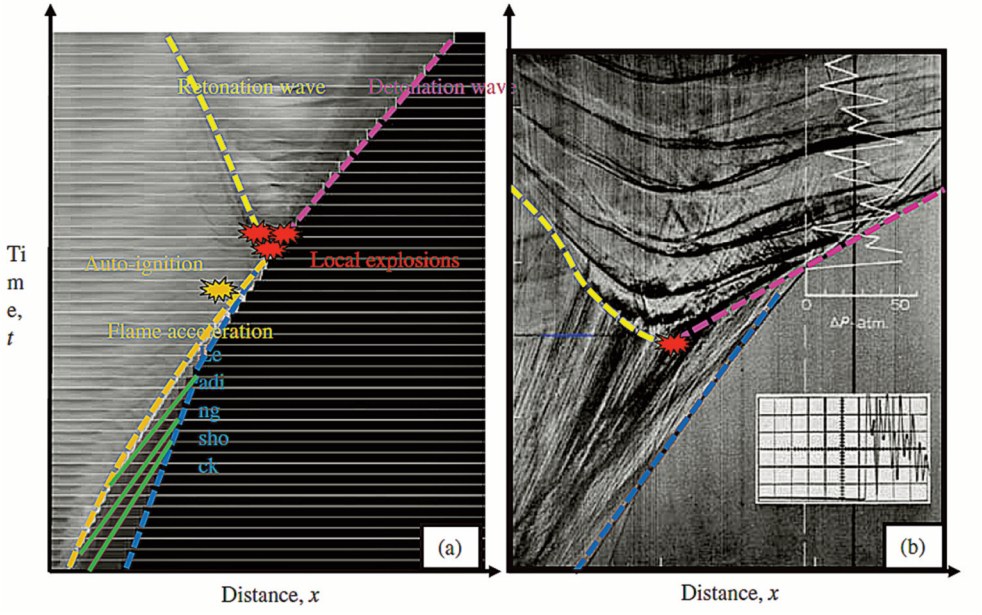


Fig. 8. The *x–t* diagrams of the DDT process: (a) results of this simulation and (b) experimental results (Urtiew and Oppenheim, 1966 [12]). In both diagrams, the horizontal axis shows the distance from the left end wall of the tube, while the vertical axis shows the time (courtesy of Machida et al. [20]).

5. 3-D VISUALIZATION OF THE DDT

Recently, at the A.V. Luikov Heat and Mass Transfer Institute in Minsk, serious research has been directed towards a better understanding of the nature of DDT in gaseous mixtures. They built special instrumentation to observe stereoscopic pictures of self-illumination in a cylindrical optically transmitting tube. The studies were carried out for oxy-acetylene mixtures with argon and nitrogen dilution respectively. The test stand was equipped with two identical high-speed monochrome Photron Fastcam SA-Z type 2100 cameras; they were installed in one cross section of the tube, at an angle of 90 degrees to each other. Both cameras were equipped with Edmund Optics BP 430 nm × 10 nm OD4 50 mm filters, whose spectral band corresponds to the luminosity of intermediate CH radicals. The cameras were placed in the location of the expected DDT transition, so the stereoscopic view of the region was observed in the selected spectral range and with a frequency of 200,000 f/s. This guaranteed high temporal and spatial resolution of the process observed. A detailed description of the test stand and test can be found in [9, 21]. They found that just before the DDT, the turbulent flame had a conical structure and that the ignition points, "hot spots", which trigger the DDT are always located at the annular boundary layer 6-35 mm ahead of the cone flame. This is shown in Fig. 9 and 10.

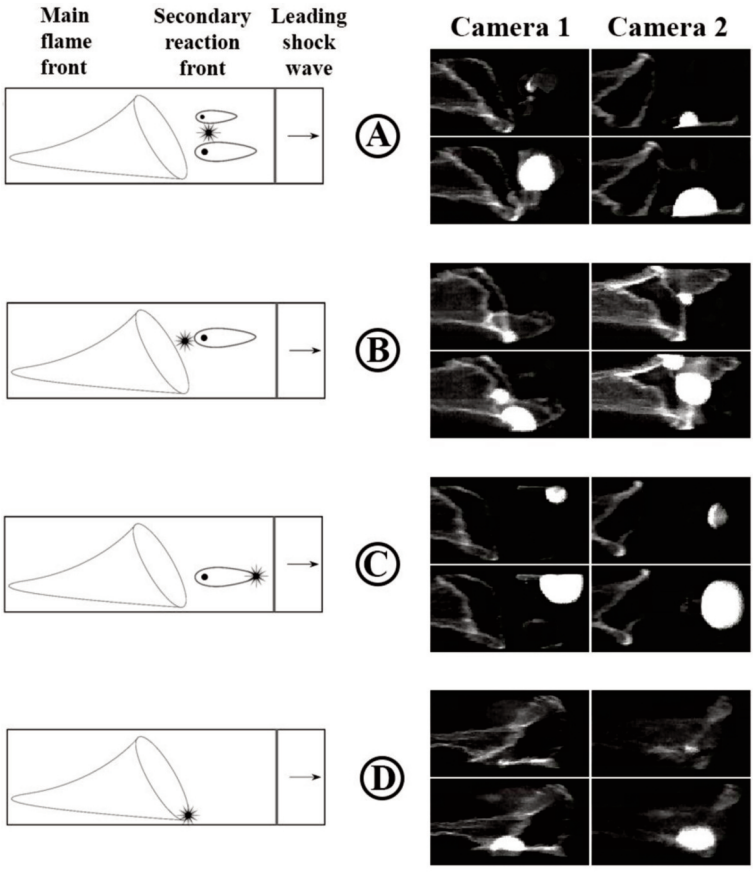


Fig. 9. Secondary auto-ignitions ahead of the flame front. The velocity of the leading shock wave M = 3 – 3.5, and for these conditions the temperature at the ignition spots is about 250–300K higher than the temperature at the center of the flow (courtesy of Krivosheyev et al. [22]).

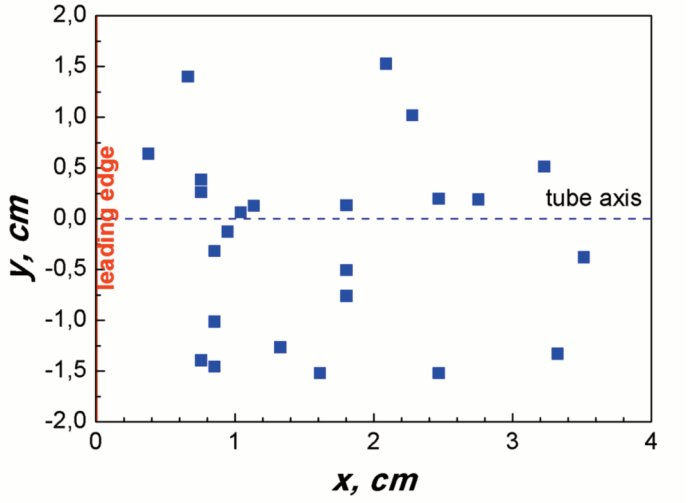


Fig. 10. Measured hot spot locations in the boundary layer as related to the position of the flame front (courtesy of Krivosheyev et al. [22]).

Simple one-dimensional calculations by the authors showed that the observed decrease in velocity in the boundary layer near the tube walls by 350 m/s will lead to a local increase in gas temperature by 250 K. This is sufficient to decrease by 15 times the ignition delay in the gas in the boundary layer behind the leading shock wave. They also estimated that the temperature in the region of a hot spot must be about 250–300 K higher than the gas temperature in the post-shock flow and indicated that this temperature rise is due to adiabatic compression. The main reason for such an temperature increase should more properly be linked to the non-isentropic processes that occur in the boundary layer due to friction and stagnation of the gas mixture initially accelerated behind the leading shock wave generated by the accelerating flame. In the conclusions, they also noted that the case of weak initiation of the DDT in a tube is not possible without the processes which happen in the boundary layer [9, 22]. Thus, it should be stated that the processes which happen in the turbulent boundary layer are always essential for the DDT in tubes for cases of weak initiation.

6. SUMMARY AND CONCLUSIONS

Gradients of mixture parameters are inherent properties of the combustion processes; it is not possible to state that there are no temperature, pressure, density or other parameter gradients as well as gradients of reaction rate, intermediate mixture composition etc. in all dynamic processes associated with combustion. If no gradients exist, the mixture remains unreacted or there are quiescent combustion products. There is no question that there is no coherent energy release in laminar or turbulent combustion as well as in detonations, not excluding all intermediate stages such as transition from laminar to turbulent combustion, origin of detonation, ignition process and flame quenching by thermal or chemical gradients. But each process, beside gradients, has the same dominant feature/mechanism which is characteristic of it. This also relates to the transition from deflagration to detonation. The most important and most characteristic feature of the DDT is the sudden abrupt change in velocity, temperature, pressure, density of propagation – it is just an "explosive" transition from subsonic to supersonic combustion. A. K. Oppenheim was the first to name this process as it is: an explosion in an already exploding mixture, so he named this process "explosion in the explosion" – which is a most appropriate and informative wording

for the description of this process. He showed this in many very beautiful laser Schlieren stroboscopic pictures of DDT in gaseous hydrogen-oxygen mixtures, which to this day continue to be the most often cited images of this sort.

In conclusion:
- transition from deflagration into detonation in a gaseous mixture happens suddenly in the form of an "explosion in the explosion",
- transition to detonation in gaseous mixtures is always associated with a strong retonation wave,
- the transition region is always located ahead of the accelerating flame front in the boundary layer,
- strong non-isentropic processes which happen in the boundary layer are responsible for a local temperature increase which leads to self-ignition and a local explosion which trigger detonation,
- no DDT could happen in tubes/channels without boundary layer interaction with flow generated ahead of the accelerating flame,
- the gradual transition from deflagration into detonation is only observed for gaseous mixtures with large concentrations of large inert particles.

Recently conducted research on different aspects of detonation initiation in gaseous mixtures have yielded new insight into this process, already under study for more than a half century. Better understandings of the DDT in gaseous mixtures will help us to organize initiation of detonation more easily, and in other ways to prevent its development in situations where such processes could be very destructive in industry and mining, which can result in casualties and property damage.

Acknowledgments: It should be mentioned that all three authors were considered by A.K. Oppenheim as his "scientific sons" and all were honored with the Oppenheim Prize awarded by the Institute of Dynamics of Explosions and Reactive System (IDERS), USA. The calculation of ignition in the boundary layer ahead of an accelerating flame was first obtained numerically by Edyta Dzieminska in her PhD. thesis conducted at the Aoyama Gakuin University under the supervision of Professor A.K. Hayashi. The proof of ignition in the boundary layer ahead of the accelerating flame was provided by the team of scientists from the A.V. Luikov Heat and Mass Transfer Institute, in Minsk directed by Academician Oleg Penyaskov. This paper was written in memory of A.K. Oppenheim's contribution to DDT research. A.K. Oppenheim was born in Warsaw in 1915, graduated from the Warsaw University of Technology (*Politechnika Warszawska*), received an honorary doctorate from his Alma Mater, and was a foreign member of the Polish Academy of Sciences.

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