Extinguishing detonation in pipelines – optimization of the process.

Z. A. Walenta, A. M. Słowicka
Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland

1. Introduction

The necessity of extinguishing detonation, which may occur in pipelines transporting gaseous fuels, is nowadays a very important technological problem. The standard devices used for it consist of matrices of very narrow channels. Cooling the gas by cold walls of such channels may extinguish the flame and stop detonation. Detonation may also be extinguished if the cross-section of the channel transporting gas increases abruptly at some place. The desired effect may be achieved if the generated rarefaction waves decrease sufficiently the temperature of the flame (Teodorczyk et al. 1988, Cai et al. 2002, Dremin 1999, Walenta et al. 2004). It might be expected, that simultaneous use of both methods – using narrow channels with variable cross-section – should give even better results. Additional profit might come from the fact, that the flow in narrow channels is usually laminar; the abrupt increase of the cross-section would introduce some turbulence and this way enhance cooling by the walls. However, if the cross-section of the channel increases and decreases, the unwanted heating of the gas may occur. To estimate the net result, which is not obvious, it is necessary to perform suitable simulations and experiments. The present paper is devoted to numerical simulation of the phenomenon.

2. Method of simulation

The simulations presented in this paper were performed with the Direct Simulation Monte – Carlo (DSMC) technique (Bird 1994). This technique makes it possible to simulate flows in various geometrical configurations and, apart from that, it offers a possibility of taking into account the relaxation phenomena and chemical reactions (Larsen et al. 1974, Bird 1994). This, unfortunately, increases complexity of the computer programs and the necessary computing times. However, in the considered case considerable simplifications can be made because in a detonation wave the medium is far from thermodynamic equilibrium, combustion proceeds very fast and the relaxation processes at the molecular level may therefore be disregarded. The factor of prime importance, which remains, is the produced thermal energy.

2.1. Model of a detonating medium

As always in the Direct Monte – Carlo simulations the medium is treated as an ensemble of molecules, colliding with each other and with walls and moving along straight lines with constant speed between collisions. Since in the present work only the influence of the shape of the channel upon the process of extinguishing detonation is investigated, a very simple model of the detonating medium (Walenta et al. 2004, 2008) may be used. It is assumed, that all molecules of this medium are identical, hard spheres. Part of them, uniformly distributed in space, carry certain amount of "internal" energy (of unspecified character). This energy may be transformed into kinetic energy during collisions with molecules, which carry no "internal" energy (belong to those, which can carry no energy), provided that the two colliding molecules approach each other with sufficiently high velocity (see Figure 1 for definition of "velocity of approach"). The relative velocity of the molecules after collision is then increased suitably. The "internal" energy may be released either in the first collision of this kind (no delay), or during some later collisions (delayed energy release). A molecule which had lost its "internal" energy may regain it in collision with another molecule if their "velocity of approach" is higher than velocity corresponding to this "internal" energy (the "inverse reaction"). The relative velocity of the molecules after collision is then decreased suitably.

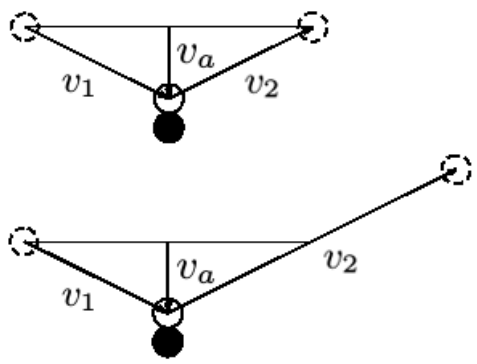

Figure 1. Collision of two molecules in reference frame connected with one of them: upper – elastic, bottom – with energy release; v_1 – relative velocity of the molecules before collision, v_2 – relative velocity after collision, v_a – "velocity of approach" of the molecules.

2.2. Interactions with solid walls

To simulate the interactions of the molecules with solid walls the very simple model introduced by J.C. Maxwell (Maxwell 1952) has been employed: molecules reflect from the walls either specularly (without exchange of tangential momentum and energy) or diffusely (molecules are adsorbed by the wall and re-emitted in directions selected at random with energies corresponding to temperature of the reflecting wall). The ratio of the number of molecules reflected diffusely to the to-

tal number of the reflected molecules (called "accommodation coefficient", α) may vary from the value 0 to 1. The value $\alpha = 0$ (purely specular reflections) corresponds to no exchange of tangential momentum and energy, the value $\alpha = 1$ corresponds to maximum possible exchange (maximum friction and cooling). For the majority of the so-called "technological surfaces" the accommodation coefficient is close to unity.

2.3. Details of calculations

Here we present the results of simulations of the behaviour of a detonation wave in three channels of different geometries, in the medium containing different percentages of the molecules "carrying energy". The energy, carried by a single molecule and released in a collision, was always such, that the relative velocity of the colliding molecules was increased by the value equal to 10 times the most probable molecular speed. The "threshold velocity" of approach of the colliding molecules, necessary to release the "internal energy", was equal to about 5.48 times the most probable molecular speed.

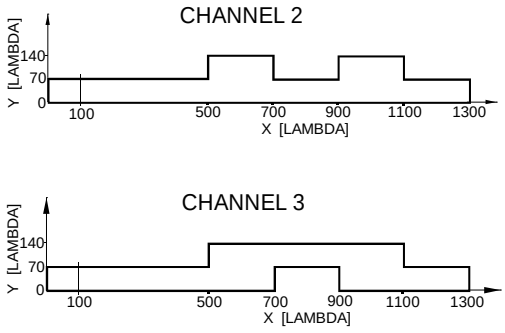

Figure 2. Shapes of the channels 2 and 3. Lambda – mean free path in front of the wave.

Channel 1 was of standard geometry (straight, rectangular cross-section of costant area); its length was equal to 1200 units and its cross-section was 70x70 units, where the unit of length was equal to 1 mean free path of the molecular motion in front of the detonation wave. The interior of the channel was divided into 5880000 cubic cells of dimension equal to 1 unit of length. Each cell contained, about 5 molecules. Channels 2 and 3 are shown schematically in Figure 2. The width of each channel was constant and equal to 70 units. All other dimensions are given in the figure. The interior of each channel was divided into cubic cells of dimension equal to 1 unit – similarly to channel 1. Each cell contained, as before, about 5 molecules. The wave was initiated by instant removal of a "diaphragm", placed at $x = 100$ units. The temperature of the driver gas (behind the diaphragm) was 10 times higher than that of the driven gas. The pressure was such, that after the diaphragm removal the shock wave of Mach number $Ms = 2$ was produced. At the beginning and the end of each channel, i.e. for $x < 400$ units and $x > 1000$ units in channel 1 and for $x < 500$ units and $x > 1100$ units in channels 2 and 3 the molecules were reflected from the walls specularly, i.e. without exchange of tangential momentum and energy. Such region of flow without losses at the beginning of the channel was necessary for the detonation to develop. The flow without losses at the end of the channel was assumed to check whether the extinguished detonation would not reappear. The simulations were performed for a number of different percentages of the "energetic" molecules in the medium in front of the diaphragm. The Table 1 presents these percentages for all channels considered in this investigation.

Table 1. Percentages of molecules carrying "internal" energy in the three considered channels.

Number of channel	Percentage of molecules carrying "internal" energy (%)
1	20, 21, 22
2	25, 26, 27
3	26, 27, 28

3. Results

The results of the performed simulations are presented in the following figures. Each of them contains several diagrams of temperature distribution (averaged over the local cross-section) along the channel, for different time intervals from removing the diaphragm, superimposed upon one another. The diagrams of temperature have been selected, because distribution of this parameter is very characteristic for the detonation wave and makes it easy to recognize its presence. The first three figures show the results for channel 1 (Figures 3,4,5), the next three – for channel 2 (Figures 6,7,8), the last – for channel 3 (Figures 9,10,11).

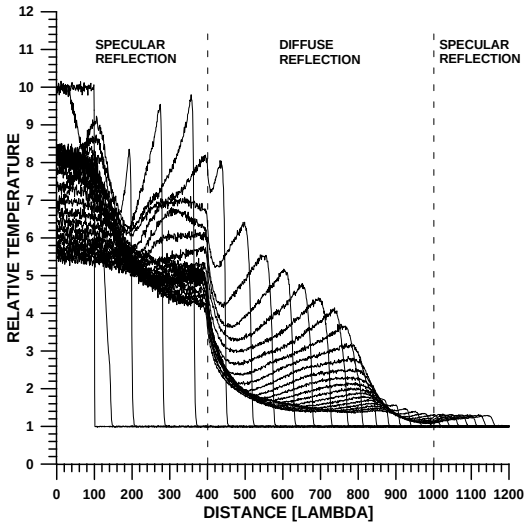

Figure 3. Detonation in channel 1, in the medium containing 20% of "energetic molecules". Lambda – mean free path in front of the wave.

3.1. Channel 1

In Figure 3 the diagrams of temperature inside the channel 1 for the medium containing 20% of "energetic" molecules are presented. After the diaphragm removal the detonation wave is formed. It then speeds up, increases its intensity, and subsequently enters into the area where molecules reflect from the channel walls diffusely, the "burning" gas is cooled down and the flame disappears. The detonation wave is transformed into shock, which is weak and seems to decay gradually.

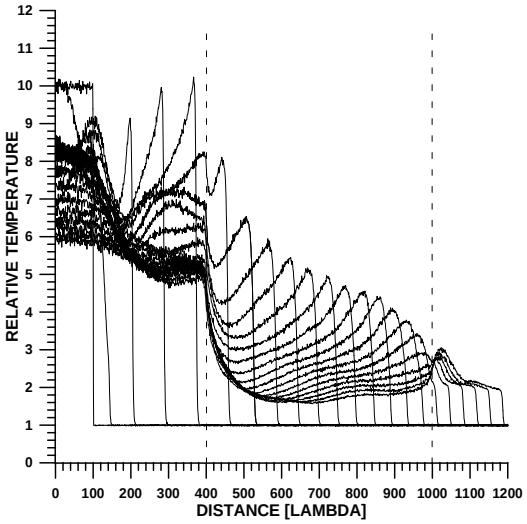

Figure 4. Detonation in channel 1, in the medium containing 21% of "energetic molecules". Lambda – mean free path in front of the wave.

Figure 4 shows similar diagrams for the medium containing 21% of "energetic" molecules. The general picture is very close to that shown in Figure 3, however the shock emerging at the end of the channel is much stronger and it is not certain whether it would not transform back into the detonation wave.

Figure 5 shows finally the situation for the medium containing 22% of "energetic" molecules. In the central part of the channel, where friction and heat exchange at the walls are present, the detonation wave only becomes weaker, but retains its character. After entering the area of no friction and cooling it returns back to its former intensity and speed. From the above results the conclusion may be drawn, that 21% is the limiting amount of "energetic" molecules (as defined above) in the "detonating medium", below which the detonation may be extinguished in channel 1.

3.2. Channel 2

In Figure 6 the diagrams of temperature inside the channel 2 for the medium containing 25% of "energetic" molecules are presented. Formation of the detonation is here similar to that in the previous case, only the speed and intensity of the wave are much higher. The passage to the area of increased cross-section and diffuse reflection of molecules from walls cause appreciable decrease of

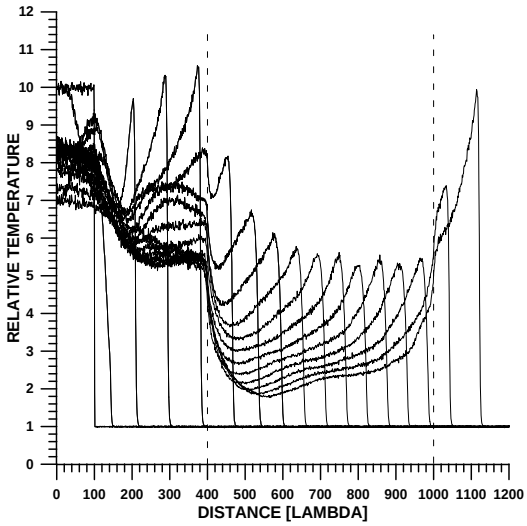

Figure 5. Detonation in channel 1, in the medium containing 22% of "energetic molecules". Lambda – mean free path in front of the wave.

temperature. The detonation, however, quickly regains its character, only its speed and intensity are lower than before. The passage into the next, narrower part of the channel influences it very weakly.

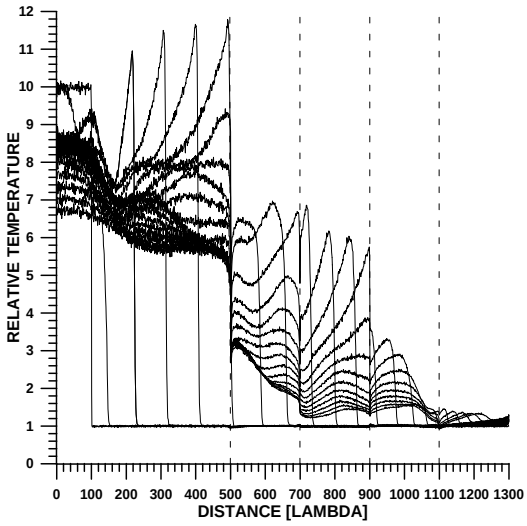

Figure 6. Detonation in channel 2, in the medium containing 25% of "energetic molecules". Lambda – mean free path in front of the wave.

The passage to the second area of increased cross-section causes next decrease of temperature which, together with heat exchange and friction at the walls, leads to extinguishing the flame and damping the detonation, so that only very weak shock passes to the last, narrow part of the channel. It should be noted, that there is no visible increase of temperature at any of contractions of the channel, which seems surprising.

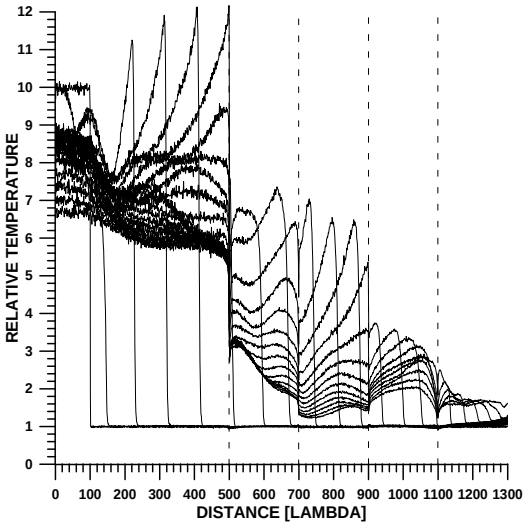

Figure 7. Detonation in channel 2, in the medium containing 26% of "energetic molecules". Lambda – mean free path in front of the wave.

Figure 7, for the medium containing 26% of "energetic" molecules, is very similar to the previous one. All waves are only slightly stronger and faster. It applies, in particular, to the shock emerging at the end of the channel – it is not certain if later it would not transform back into the detonation wave.

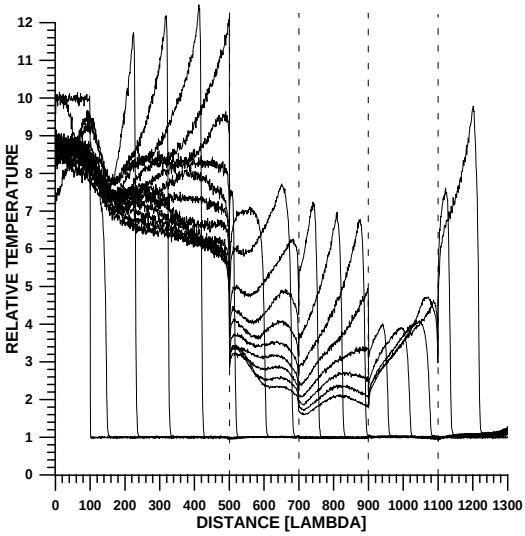

Figure 8. Detonation in channel 2, in the medium containing 27% of "energetic molecules". Lambda – mean free path in front of the wave.

Figure 8 shows the case of the medium containing 27% of "energetic" molecules. Here the detonation wave is only slightly stronger than that, shown in Figure 7, still it retains its character all the time and in the last part of the channel (without friction and heat exchange at the walls) it quickly regains its initial intensity. From the results presented above it may be concluded, that channel 2 is capable of extinguishing detonation in the medium containing no more than 26% of "energetic" molecules.

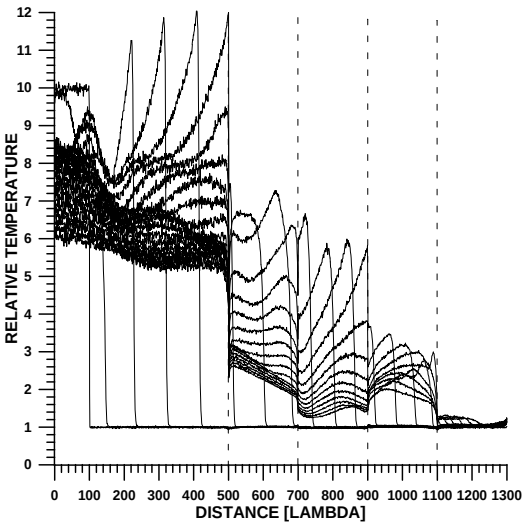

Figure 9. Detonation in channel 3, in the medium containing 26% of "energetic molecules". Lambda – mean free path in front of the wave.

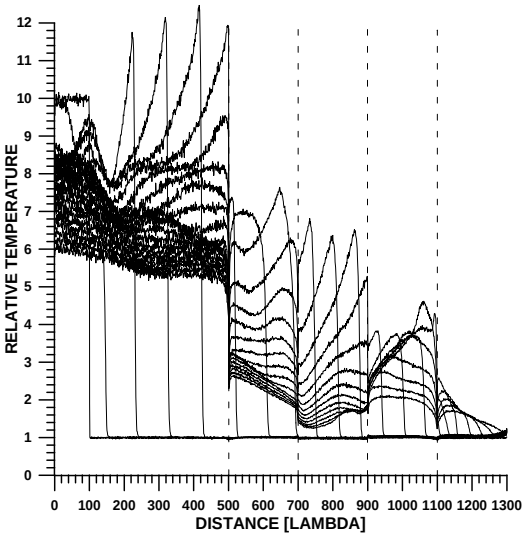

Figure 10. Detonation in channel 3, in the medium containing 27% of "energetic molecules". Lambda – mean free path in front of the wave.

3.3. Channel 3

The behaviour of detonation wave in channel 3 (see Figures 9, 10, 11) seems to be very close to the described above for channel 2. They differ only slightly in efficiency: channel 3 is capable of extinguishing detonation in the medium containing no more than 27% of "energetic" molecules (instead of 26% for channel 2). This may be due to the fact, that the flow in channel 3, apart from expansions and contractions, must do several turns which may additionally increase the level of tur-

bulence of the flow and enhance the heat exchange with the walls.

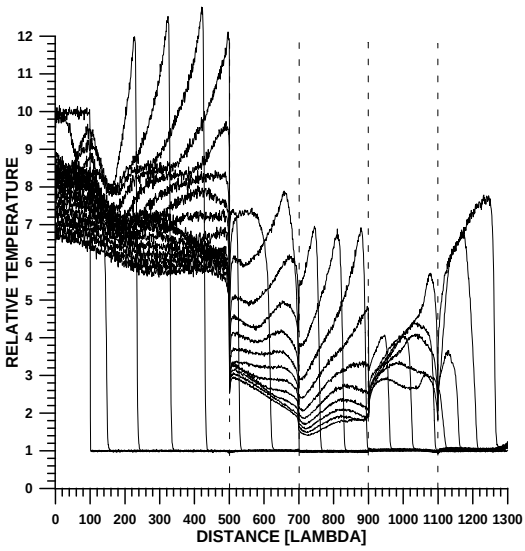

Figure 11. Detonation in channel 3, in the medium containing 28% of "energetic molecules". Lambda – mean free path in front of the wave.

4. Discussion and conclusions

The presented simulation results look very promising, as far as increasing efficiency of devices for extinguishing detonation in pipelines is concerned. However, it must be kept in mind, that:

- the simulations were performed for a strongly simplified model of the detonating medium
- the dimensions of the considered channels were very small, which was connected with limited capacity of the available computers. It is not obvious, that at larger scale the results will be equally good.
- the channels of the suggested shapes may create big resistance to the flow. To overcome that it may be necessary to increase their cross-sections, which would decrease the efficiency of the device so that the net result may not be worthwhile.

At the present stage it seems necessary to make experiments validating the performed simulations. The work is still in progress and we hope to be able to present more results in the future.

References

Bird G.A.: Molecular gas dynamics and the direct simulation of gas flows, Clarendon Press, Oxford, 1994.

Cai P., Hoshi S., Obara T., Ohyagi S., Yoshihashi T.: Diffraction and re-initiation of detonations behind a backward–facing step, Shock Waves, 12, 221–226, 2002.

Dremin A.N.: Toward detonation theory, Springer, 1999.

Larsen P.S., Borgnakke C., in Rarefied Gas Dynamics (ed. M. Becker and M. Fiebig), 1, Paper A7, DFVLR Press, Porz–Wahn, Germany, 1974.

Maxwell J.C.: The scientific papers of James Clerk Maxwell (W.D. Niven, ed.) New York: Dover, 2, 706, 1952.

Teodorczyk A., Lee J.H.S., Knystautas R.: Propagation Mechanism of Quasi-Detonations, Proceedings of the Combustion Institute, vol.22, pp. 1723–1731, 1988.

Walenta Z.A., Teodorczyk A., Dabkowski A., Witkowski W.: Direct Monte – Carlo simulation of a detonation wave in a narrow channel, containing flammable gas, Central European Journal of Energetic Materials, 1(1), 49–59, 2004.

Walenta Z.A., Lener K.: Direct Monte – Carlo simulation of developing detonation in gas. Shock Waves, 18, 71–75, 2008.