Detonation Waves in Narrow Channels of Various Shapes

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Abstract: One of the important contemporary technological problems is connected with necessity of extinguishing detonation, which may occur in pipelines transporting gaseous fuels. To achieve this goal usually a matrix of very narrow channels is placed inside the pipeline, perpendicularly to its axis. In our recent paper (Walenta and Slowicka (2016)) we have shown, that channels with sharp changes of cross-section should be more efficient in this respect than traditionally used straight channels with constant cross-section area. In this paper we demonstrate how detonation behaves in the channels, in which gas flows under realistic conditions – when friction and heat exchange are present. We take into account the fact, that gas flowing through such channels accelerates and its density decreases considerably.

Key words: detonation waves, detonation damping, narrow channels

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1. Introduction

The necessity of extinguishing detonation, which may occur in pipelines transporting gaseous fuels, creates nowadays a very important technological problem. The standard devices used for this purpose 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 is achieved if the generated rarefaction waves decrease sufficiently the temperature of the flame (Teodorczyk et al. (1988), Dremin (1999), Cai et al. (2002), Walenta et al. (2004)). It has been shown, that simultaneous use of both methods – using narrow channels with variable cross-section may give even better results (Walenta and Slowicka (2016)). Additional profit would come here from the fact, that the flow in narrow channels is usually laminar; the abrupt change of the cross-section introduces some turbulence and this way enhances cooling by the walls. There are, however some doubts connected with the results presented in the paper (Walenta and Slowicka (2016)). First: channels of the suggested shapes may create big resistance to the flow. To overcome that it might be necessary to increase their cross-sections, which would decrease the efficiency of the device so that the net result might not be worthwhile. Second: it is not clear how detonation waves would behave in the environment with variable parameters – particularly density and velocity. The present paper is devoted to clarification of these problems. The method used for this purpose is the numerical simulation with the DSMC technique.

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2. Method of simulation

The simulations presented in this paper were performed with the standard Direct Simulation Monte–Carlo (DSMC) technique (Bird (1994)). The DSMC technique makes it possible to simulate flows in various geometrical configurations and it also offers a possibility of taking into account the relaxation phenomena and chemical reactions (Larsen and Borgnakke (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 be disregarded. The factor of prime importance is the produced thermal energy.

3. Model of a detonating medium

In the present work we investigate only the influence of shape of the channel upon the flow inside it and upon the process of extinguishing detonation, therefore a very simple model of the detonating medium (Walenta et al. (2004), Walenta and Lener (2008)) could be used. It has been 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). The remaining molecules are "inert" – they can carry no "internal" energy and cannot accept it in any way. The "internal" energy of a molecule may be transformed into kinetic energy during collision with an "inert" molecule, provided that the colliding molecules approach each other with sufficiently high "velocity of approach" (Fig. 1 – left).

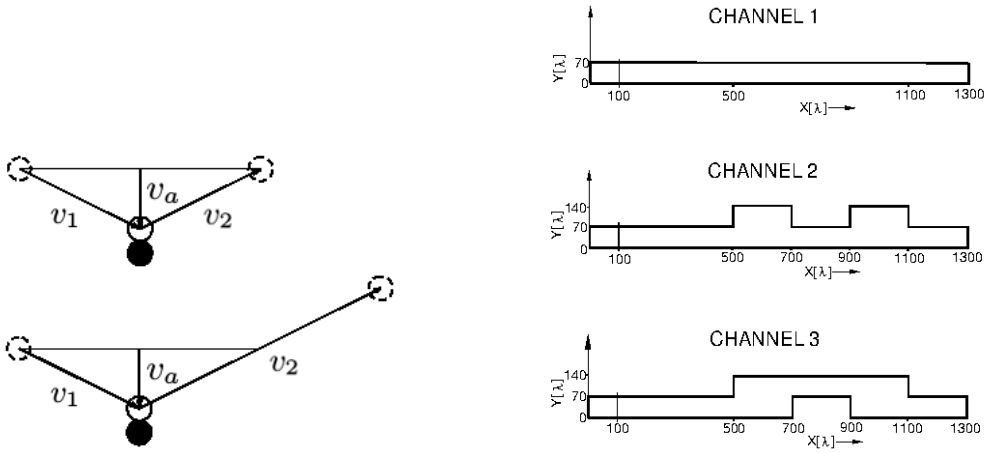

Figure 1. Left: collisions of two molecules in reference frame connected with one of them. Top – elastic, bottom – with energy release; v_1 – relative velocity before collision, v_2 – relative velocity after collision, v_a – "velocity of approach". Right: shapes of the considered channels (λ – mean free path at the initial conditions).

The relative velocity of the molecules is then increased suitably. A molecule which had lost its "internal" energy may regain it in a collision with an "inert" molecule if their "velocity of approach" is higher than velocity corresponding to this "internal" energy. The relative velocity of the molecules is then decreased suitably. The assumed "internal" energy of a single molecule 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.

4. Interactions with solid walls

To simulate the interactions of the molecules with 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 total number of the reflected molecules (called "accommodation coefficient", α) may vary from 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 majority of the so-called "technological surfaces" the accommodation coefficient is close to unity.

5. Details of simulations

We present the results of simulations of the behaviour of the stationary flow and detonation waves in three channels of different geometries (Fig. 1 – right), similar to those considered in (Walenta and Slowicka (2016)). The fourth channel considered in that paper (channel 2, with inclined walls) was not investigated here, since it had been found to be worse than other two channels with changes of cross-section.

Channel 1 (Fig. 1 – right) was straight, of constant, rectangular cross-section 70x70 units and length 1300 units (the unit of length was equal to 1λ – mean free path of the molecular motion at the initial conditions). The width of the other two channels was equal to 70 units; other dimensions are given in Fig. 1 – right.The interior of each channel was divided into cubic cells of dimension equal to 1 unit. Each cell contained initially about 5 molecules. In each channel, 100 units from its left end, there was a "diaphragm" separating the hot driving gas from the rest of the channel. The temperature of the driving gas was 10 times higher than temperature of the gas behind the "diaphragm". The pressure was such, that after removing the "diaphragm" the shock wave of Mach number 2 was generated. At both ends of each channel, i.e. for $x < 500$ units and $x > 1100$ units the molecules were reflected from the channel walls specularly, i.e. without exchange of tangential momentum and energy. Such region of flow without losses behind the "diaphragm" was necessary for the detonation to develop. The flow without losses at the end of the channel was assumed to enable checking whether the extinguished detonation would not reappear. In the central part of each channel, i.e. for $x > 500$ units and $x < 1100$ units the molecules were reflected from the walls diffusely, i.e. with maximum friction and cooling.

The simulation was performed in two stages. During the first one – generation of the stationary flow – the molecules were allowed to escape freely from the right end of the channel, however all escaping molecules were transferred to the place at the right side of the "diaphragm". This created certain density and pressure differences and, after sufficient time (not less than 100000 steps – about 90 hours of computing time) it led to establishing stationary flow. The second stage was initiated by the "diaphragm" removal. It produced the shock wave, which subsequently was transformed into a detonation wave.

The simulation for each channel was performed only once, for the percentage of "combustible" component (molecules carrying "internal" energy), for which detonation was extinguished according to the results of (Walenta and Slowicka (2016)).

6. Results

6.1. Stationary flow

The results of simulation of stationary flow in all three considered channels are shown in Fig.2. The distribution of density along the channel is shown in Fig. 2 (upper, left), velocity – in Fig.2

(upper, right), pressure – in Fig. 2 (lower, left), and flow rate in Fig. 2 (lower, right). Density and pressure are related to their initial values (before beginning of the flow). Velocity is related to the initial value of the most probable velocity of the molecular motion. All parameters are averaged over the local cross-section of the channel. The horizontal part of each line, in the range $100 < x < 500$, corresponds to flow in the channel without friction and cooling.

From the abovementioned figure it may be concluded, that variation of each of the stationary flow parameters: density, velocity and pressure along the channel is appreciable. It may be expected, that it would affect the appearing detonation wave. There is, however, one additional important point. The pressure drop along channel 1 is larger than that along channels 2 and 3 (Fig. 2, lower, left). At the same time, the flow rate in channel 1 is smaller than in other two channels (Fig. 2, lower, right). This means, that contrary to expectations, resistance to the flow in both channels, 2 and 3, is smaller than in the straight channel 1. The probable reason is, that in the flow through very narrow channels the resistance due to viscosity is more important than resistance connected with the changes of the cross-section.

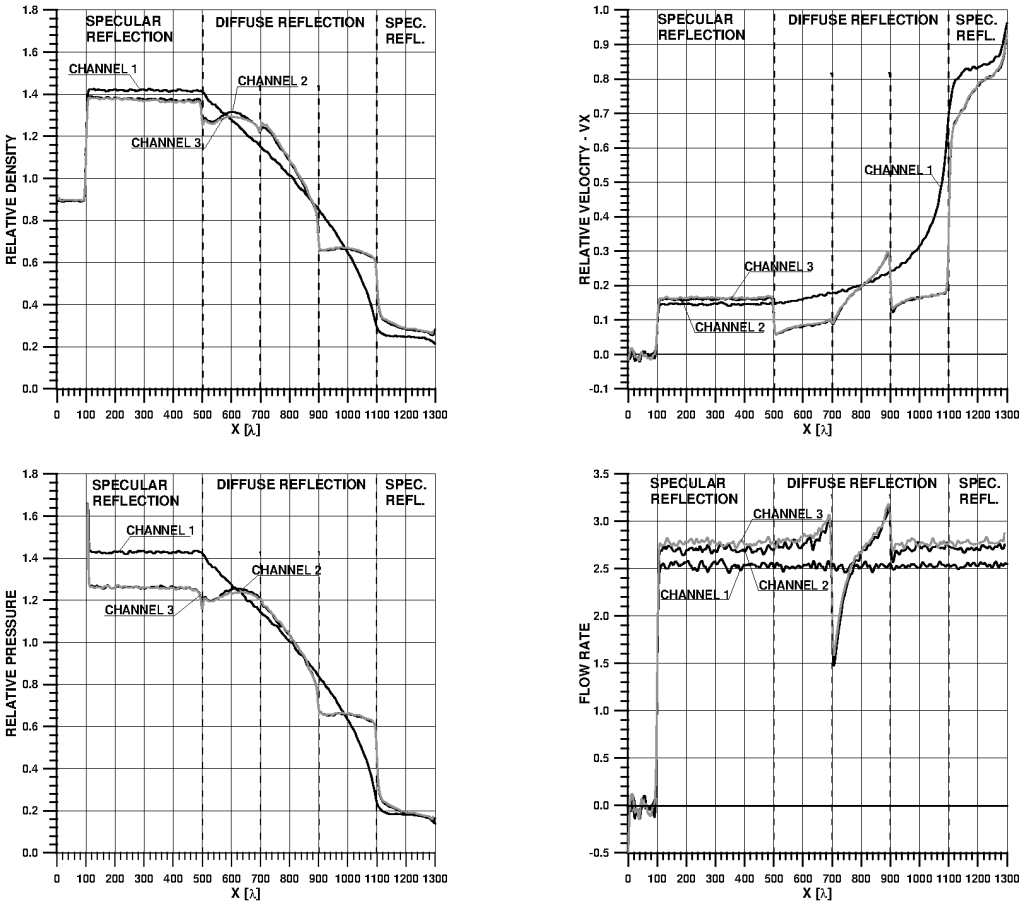

Figure 2. Distributions of parameters along the channel in stationary flow. Upper, left – density; upper, right – velocity; lower, left – pressure; lower, right – flow rate

6.2. Detonation

In this section we present the diagrams of temperature along the channel, uniformly distributed in time, resulting from simulation of the behaviour of a detonation wave in the stationary flow inside all three considered channels.

In Fig. 3 (upper, left), the diagrams of temperature inside the channel 1 (straight), for the medium containing 20% of "energetic" molecules, are shown. (For such percentage of "energetic" molecules, under no-flow conditions (Walenta and Slowicka (2016)), the detonation was extinguished).

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 then cooled down and the flame disappears. The detonation wave is transformed into weak shock, which seems to decay gradually.

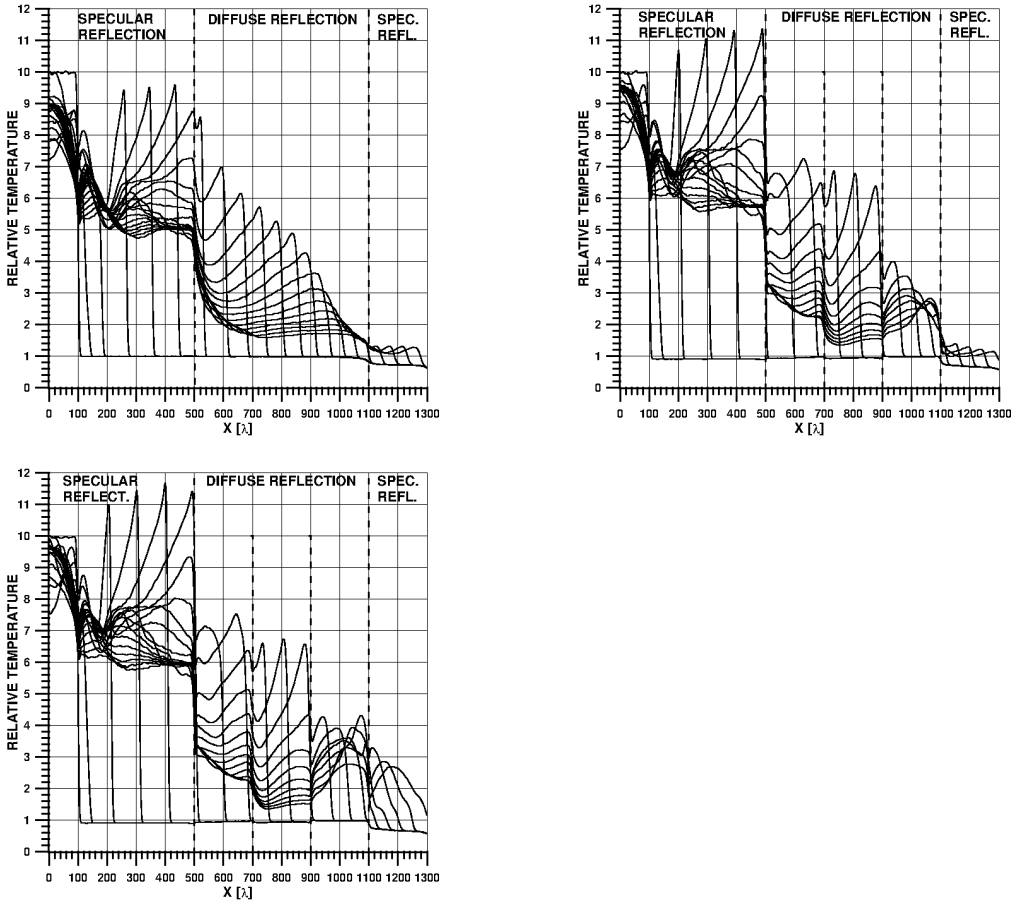

Figure 3. Temperature distributions in the channels with detonation waves progressing into stationary flow. Upper, left – channel 1 – 20% of "energetic" molecules; upper, right – channel 2 – 25% of "energetic" molecules; lower, – channel 3 – 26% of "energetic" molecules

In Fig. 3 (upper, right) the diagrams for the medium containing 25% of "energetic" molecules inside the channel 2 are presented. Formation of the detonation is here similar to that in the previous case, only the speed and intensity of the wave are higher. The passage to the area of increased cross-section and diffuse reflection of molecules from walls causes appreciable decrease of temperature. The detonation then quickly regains its character, only its speed and intensity are lower than before. The passage into the next, narrower part of the channel causes slight, but distinct decrease of the intensity of the detonation wave, as well as the temperature of the gas behind it. 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 weak shock

wave passes to the last, narrow part of the channel.

In Fig. 3 (lower) the diagrams for the medium containing 26% of "energetic" molecules inside the channel 3 are presented. The picture of the phenomenon up to the second increase of cross-section is here similar to that in the previous case, only the speed and intensity of the wave are slightly higher. This, however is sufficient for the flame not to be extinguished either in the second area of increased cross-section, or in the narrow part at the end of the channel. As the result, the intensity of the shock wave, which enters this narrow part of the channel, is increasing with time and therefore it may be expected, that this shock will be transformed back into detonation.

7. Conclusions

- It has been found, that abrupt changes of cross-section of very narrow channels do not increase the resistance to the flow, as compared to straight channels of constant cross-section.
- It has been found, that stationary flow through the very narrow channels does not influence appreciably their efficiency of extinguishing detonation.
- The remaining problem to be solved – the influence of the geometric scale of channels of the detonation damper on its efficiency – is still open. We hope to be able to solve it in the nearest future.

Bibliography

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

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

Dremin A.N. (1999). *Toward detonation theory*. Springer.

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

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

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

Walenta Z.A., Teodorczyk A., Dabkowski A., Witkowski W. (2004). 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.

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

Walenta, Z.A., Slowicka, A.M. (2016). *Extinguishing detonation in pipelines – optimization of the process*. In K. Kontis (Ed.), Proceedings of 22nd Int. Shock Interaction Symposium, Glasgow, 202–206.