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Direct Monte-Carlo Simulation of a Detonation Wave in a Narrow Channel, Containing Flammable Gas

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Abstract: The research on gaseous detonation has recently become a very important issue, mainly due to safety reasons in connexion with increasing importance of gaseous fuels. To simulate detonation, the Direct Monte-Carlo Simulation technique has been used. This technique is known to be a very powerful tool for solving complex flow problems.

Simple model of molecular collisions, making it possible to increase the thermal energy of gas in a way similar to the processes in the flame has been proposed. This model is capable of producing waves, having the features characteristic for detonation waves. Finally the efficiencies of two known methods of extinguishing detonation: cooling the gas by cold channel walls and cooling by an expansion wave have been checked.

Keywords: detonation, Monte-Carlo Simulation

Introduction

The research on detonation in gases has recently become a very important issue because of increasing importance of gaseous fuels. The urgent technological problem is connected with detonation in pipelines and the necessity of extinguishing it. This is most frequently achieved by forcing the detonation wave to pass through a system of very narrow channels. Cooling the gas by cold walls of such channels may extinguish the flame and stop detonation.

The obvious choice for the technique of simulating phenomena in narrow channels seems to be the Direct Monte-Carlo Simulation (DMCS) technique [1]. It has proven to be a very powerful tool for simulating flows in various geometrical configurations. It offers also a possibility of taking into account the relaxation phenomena and chemical reactions [1, 2], these unfortunately increase complexity of the computer programs and the necessary computing times. However, considerable simplifications can be made here thanks to the fact, that in a detonation wave combustion proceeds at large departure from thermodynamic equilibrium and at very high rate, therefore all relaxation processes at the molecular level may be disregarded. The only important factor, that remains, is the produced thermal energy.

Model of a combustible gas

As always in the Direct Monte-Carlo Simulations the gas is treated as an ensemble of molecules, colliding with each other and with walls and moving along straight lines with constant speed between collisions. The details of the numerical technique are, perhaps, best described by Bird [1].

It has been assumed, for simplicity, that all molecules are identical, hard spheres. Moreover, part of the molecules, uniformly distributed in space, carry certain amount of "internal" energy (of unspecified character), the same for each of them. This may be transformed into kinetic energy during collision with another molecule (carrying no energy), provided that the two colliding molecules approach each other with sufficiently high velocity (see Figure 1a for definition of "velocity of approach"). If this is the case, the relative velocity of the molecules after collision is increased suitably (Figure 1b).

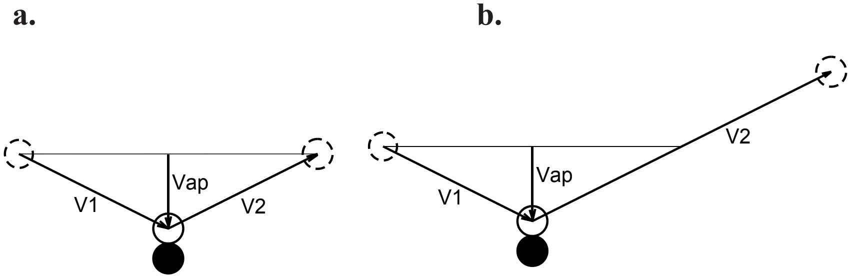

Figure 1. Collision of two molecules in reference frame connected with one of them: a – elastic; b – with energy release,
V1 – relative velocity of the molecules before collision,
V2 – relative velocity after collision,
Vap – "velocity of approach" of the molecules.

Details of calculation

To check whether the proposed model can actually simulate the detonation wave, calculations for several geometries were performed. The standard DMCS procedure, according to Bird [1] was employed; the pairs of molecules for collisions were selected with the use of the ballot-box scheme, as proposed by Yanitskiy [3]. Here, the results for one- and three-dimensional geometries, are presented. In 1-D geometry (plane wave, no walls) the number of molecules was equal to about 8 million, in 3-D geometry (flow in a pipe) it ranged from about 3 to 8 million. The calculation area was divided into 1100 cells in 1-D geometry and 1.5 to 4 million cells in 3-D geometry. The axial dimension of a cell was equal to 1 unit of length, which in the present calculations was equal to 1 mean free path of the gas molecules in the undisturbed area. The diameter of the pipe in 3-D geometry was equal to 100 mean free paths (pipe of constant cross-section) or 50 mean free paths (initial part of the pipe with increase of cross-section).

The wave was initiated by instant removal of a “diaphragm”, placed at x = 100 units of length. The gas in front of the diaphragm contained 10 per cent of the molecules carrying “internal“ energy. The energy released in a single collision was 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.

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 $M_s = 2$ was produced.

In the case of pipe flows, for x less than 400 units (mean free paths) the molecules reflected from the walls specularly, i.e. without exchange of tangential momentum and energy. Such flow without losses at the beginning was necessary for the detonation to develop.

For larger values of x, in the case of pipe with constant cross-section the so-called “diffuse reflection” was assumed. The molecules hitting the wall stuck to it and were subsequently re-emitted, with kinetic energy corresponding in average to the temperature of the wall, in directions selected at random. Such “diffuse reflection” corresponds to maximum possible friction and heat exchange and is appropriate for most of the technologically prepared surfaces.

Results

Figures 2 to 6 show selected results of the performed simulations.

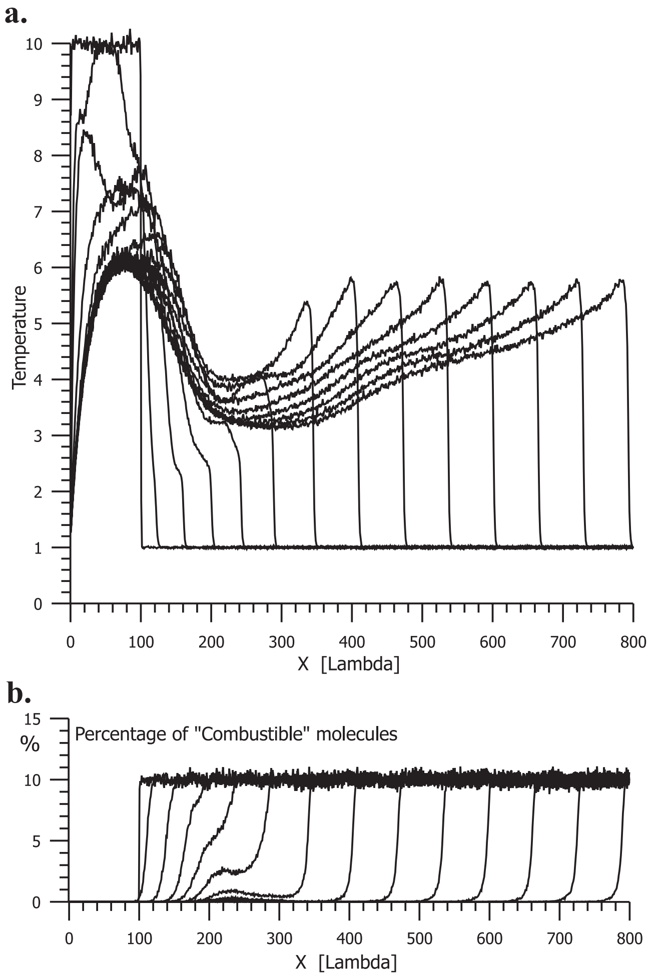

Figure 2. Formation of the planar detonation wave without influence of walls:
a – temperature distributions for 14 time instants,
b – percentage of the molecules "carrying energy".

Figures 2a and 2b correspond to the simplest case – a planar, perpendicular wave, moving along x – axis in a positive half-space, without influence of walls. Figure 2a contains distributions of gas temperature in terms of distance along the x – axis for the initial situation and for 13 subsequent instants, evenly spaced in time; Figure 2b shows the corresponding diagrams of the percentage of the "energetic component". Formation of the primary shock wave after the diaphragm removal is clearly visible. The shock then gradually speeds up and increases its intensity, which is accompanied by "burning" – decrease of the percentage of the "energetic" component. All that is the transformation into a detonation wave, which afterwards moves with constant speed and constant intensity, as expected.

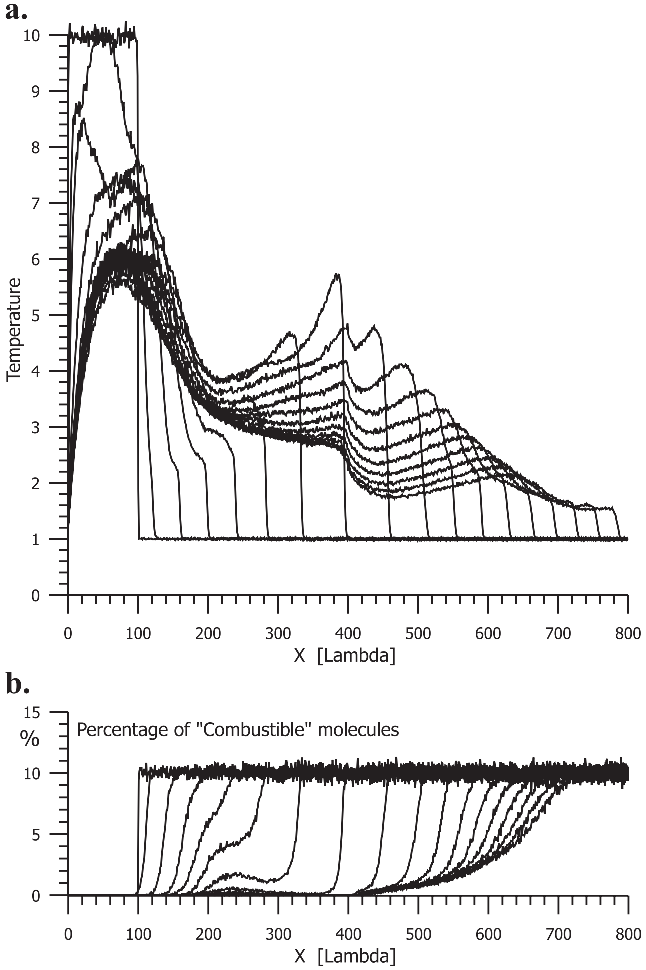

Figure 3. Formation of the detonation wave in a pipe and its decay under friction and heat exchange at the walls.

a, b – as in Figure 2.

Figures 3a and 3b show similar pictures for the wave, moving in a cylindrical pipe of the diameter of 100 mean free paths. The quantities shown there have been averaged over the cross-section of the pipe.

The left parts of the pictures, up to x = 400 lambda (area of no friction and heat exchange), look similarly to those in Figure 2 – formation of shock and detonation wave is evident. For $x > 400$, however, the walls cool the gas down, below the ignition point, and the shock moves ahead, unsupported by the flame front, getting weaker and weaker.

Figures 4a and 4b illustrate the behaviour of the detonation wave in a pipe 50 mean free paths in diameter, suddenly increasing to 150 mean free paths. The quantities shown have been averaged over the cross-section of 50 mean free paths diameter.

Formation of the shock and detonation waves, for $x < 400$ lambda, looks similarly to those in the previous cases. After passing to the area with larger cross-section the flame is extinguished by cooling in a rarefaction wave. As before, the shock moves ahead unsupported by the flame front and gradually decays.

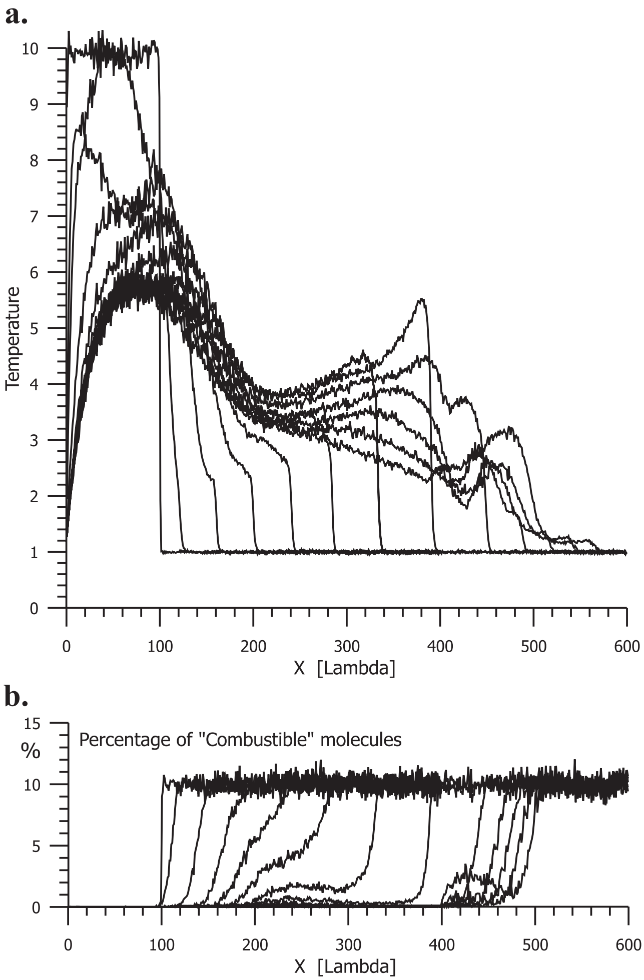

Figure 4. Formation of the detonation wave in a pipe and its decay after passing through a rarefaction wave behind sudden increase of cross-section.
a, b – as in Figure 2.

Decay of the gaseous detonation after passing through sudden increase of the channel cross-section had already been confirmed experimentally [5, 6]. Similar effect had also been observed for detonation of solid explosives

[7]. In this case it could also lead to complete extinguishing the detonation, provided that the initial diameter of the explosive was sufficiently small.

To illustrate the wave patterns inside the channels considered above the last two pictures are presented.

Figure 5 shows the lines of constant temperature in the axial cross-section of the constant-diameter pipe for one, selected position of the wave. In this picture the shock wave has already departed from the area heated by the flame. It is worth noting, that in spite of the influence of the boundary layer the shock wave is nearly plane and perpendicular to the pipe axis.

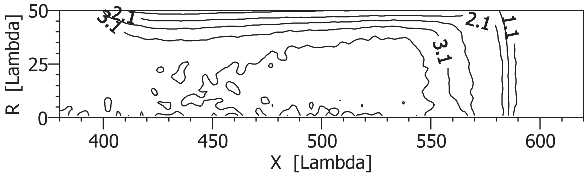

Figure 5. Momentary picture of the isotherms in a cylindrical pipe. Departure of the shock from the flame heated gas is already visible.

Figure 6 shows the lines of constant temperature in the axial cross-section of the pipe with diamater increase. The wave has already moved to the area with larger diameter – the shock has already departed from the gas heated by the flame and became very weak.

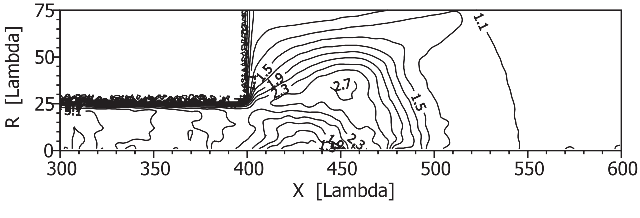

Figure 6. Momentary picture of the isotherms in a cylindrical pipe with sudden increase of cross-section.

Conclusions

A method of simulation of the detonation phenomenon, based on the Direct Monte-Carlo Simulation technique has been proposed. One of the main advantages of this method is, that it makes it possible to study detonation in narrow channels and its decay under the influence of wall friction and heat exchange. Thanks to that, this method can be used for optimizing the devices extinguishing detonation in pipelines.

The proposed model of a "detonating gas" makes it possible to increase the temperature of the gas in a simple way, simulating combustion. It has been shown, that sufficiently strong shock wave, propagating in such "detonating gas", transforms into detonation.

Two methods of extinguishing detonation have been simulated: by heat subtraction and friction at the walls of a narrow pipe and by cooling in a rarefaction wave behind sudden increase of the channel cross-section. Both methods seem to be effective; perhaps joint use of them may give the best results.

Acknowledgements

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