Multi-Processor Statistical Simulation of Forming a Gas Detonation as a Result of Quick Heating of One Tube End for Cases of Different Thresholds of a Reaction

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1 Introduction

The Monte Carlo non-stationary method of statistical simulation (MCNMSS) (another name DSMC) with weight factors [1,2] was used in calculations. It takes into account automatically all processes of heat-mass transfer. Progress in computers permits now to simulate by MCNMSS gas processes in which a local mean free path of molecules (λ) is much less than a local characteristic size of this process (L) except a small region where $\lambda \sim L$. State of gas in this region can affect sizable area of flow. Detonation in a gas is one of such processes.

2 Statement of problem and method of simulation

Non-stationary case of forming a detonation wave was considered. Simulation was carried out in the one-dimensional coordinate space and in the three-dimensional velocity space. At an initial moment, gas A was placed in the tube of constant cross-section. The gas had Maxwell velocity distribution corresponding to temperature T_1. One end of the tube was instantaneously heated and had during the process constant temperature T_w equal to $300T_1$. It was supposed that chemical reaction $A+M \rightarrow B+M$ ($M=A$ and B) took place. The ratio of molecular masses (m_i) of gases A and B was equal to 1. The same reaction was considered by Anderson and his coworkers [3, 4]. This is an analogue to the case of internal molecular energy release. The considered thresholds of the reaction (Q_{AB}) were equal to $90kT_1$, $300kT_1$, $400kT_1$ and $440\ kT_1$ (k is the Boltzmann constant). The energy release in reaction (Q) was equal to $402.6\ kT_1$. It was supposed that a collision of two particles leads to the reaction if the total energy of their relative motion is higher than the threshold of the reaction. All considered molecules were treated as hard spheres with equal diameters without internal structure. Particles reflected elastically from the cool wall at the boundary of the simulation region. It was supposed that molecules had temperature of the hot wall after collision with it (full accommodations).

Used method employs weight factors [1, 2 (see scheme 2)]. Parallel calculations were carried out by means of multi-processor computers CLICP and CLI-X of computer center in Institute of Problems of Chemical Physics. Domain decompositions of a simulation region was performed [5]. Standard Message Passage Interface (MPI) [6] was used to communicate data between processors. And 10 processors were used. The modeled region spread from 0 to $18000\lambda_1$ (λ_1 is λ at the initial moment of time). The size of spatial cell (Δx) was equal to $0.15\lambda_1$. The time of splitting of collision and displacement stages Δt was equal to $0.04\lambda_1/u$. Here u is the most probable thermal velocity of molecules with mass equal to 1 for T_1.

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3 Results

In considered case mass of reagent m_A is equal to mass of product m_B, all masses being equal to 20. And there is the Hugoniot analytical relation:

$$p_2/p_1=(4+2Q/kT_1- n_1/n_2)/(4\, n_1/n_2-1).$$

Here, indices 1 and 2 refer to parameters ahead of and behind a wave, p_i is a pressure and n_i is a numerical density of a gas. This formula is from [3].

It is easy to obtain from this analytical expression of the Chapman-Jouguet condition. If we denote $z=2Q/kT_1$ than we obtain this expression

$$n_1/n_2=\{[2(z+5)-(4z^2+15z)^{1/2}]/10\}.$$

It gives the following parameters of the Chapman-Jouguet condition for our case: n_1/n_2=0.6254, p_2/p_1=538.4, T_2/T_1=338, velocity of detonation D=6.11 u.

Fig. 1, 2 show the results of simulation for reagent A and product B respectively at the moment $2700\lambda_1/u$ for Q_{AB} =90kT_1. These and other figures show profiles of macroparameters of components: concentration (solid lines), kinetic temperature (dash lines) longitudinal velocity (dot lines) and profile of total pressure of gas mixture (dash and dot lines). One can see the developed detonation process (Fig. 2). The quasi-stationary region of the flow inside product B is formed in the leading part of detonation wave. The profile of velocity shows it clearly. The region becomes longer with time. Parameters of the flow remain constant in the quasi-stationary region: $n_2/n_1\approx$1.2, $p_2/p_1\approx$330 $T_2/T_1\approx$290. These values are approximately by 25%, 34% and 15% respectively less than for the Chapman-Jouguet condition. Detonation velocity D varies from 6.19 to 6.35. The mean value 6.32 is higher than Chapman-Jouguet velocity by 3%. This is the case of weak (low-pressure) detonation.

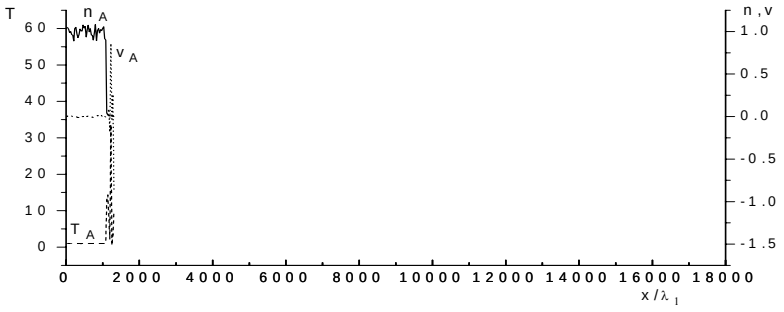

Fig. 1.

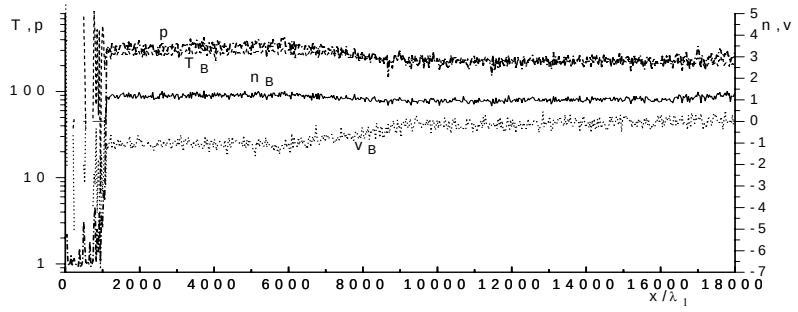

Fig. 2.

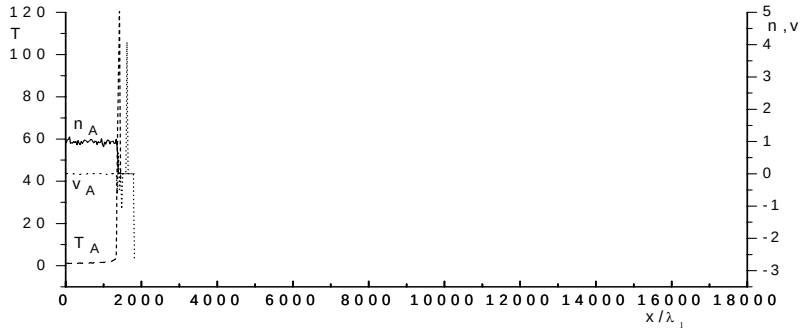

Fig. 3.

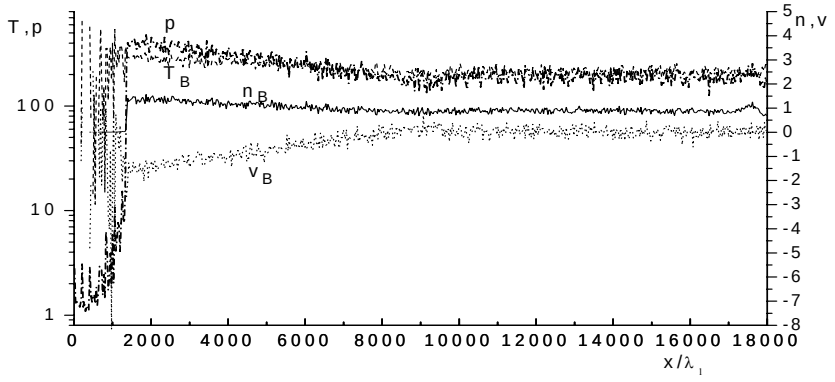

Fig. 4.

Fig. 3, 4 show the results of simulation for reagent A and product B respectively at the moment $3700\lambda_1/u$ for Q_{AB} =400kT_1. The increase of Q_{AB} changes the behavior of profiles of macroparameters. One can see disappearance of the quasi-stationary region in the leading part of detonation wave. The obtained maximum values of parameters are: $n_2/n_1\approx1.3$, $p_2/p_1\approx380$ $T_2/T_1\approx280$. Range of variation of D is from 5.06 to 5.14. The mean value 5.07 is essentially less than Chapman-Jouguet velocity (by 17%). It should be noted that detonation wave took place already at moment of time $700\lambda_1/u$.

Simulation was carried out also for Q_{AB} =400kT_1 without taken into account reaction $A+B\rightarrow B+B$. It was supposed that reaction $A+A\rightarrow B+A$ took place only. In this case, simulation was continued up to $2400\lambda_1/u$. And detonation wasn't obtained. Fig. 5, 6 show the results of simulation for reagent A and product B respectively at the moment $2400\lambda_1/u$. One can see something like a shock wave in reagent A (Fig. 5) and appearance of small amount of product B (Fig. 6). The velocity of this wave was equal to $0.76\lambda_1/u$. It should be noted a creation of region with small concentration of molecules near the hot wall. Next, simulation was carried out for the case when, as in previous case, all reaction in the beginning were taken into account and Q_{AB}=400kT_1. Then reaction $A+B\rightarrow B+B$ was excluded at moment $700\lambda_1/u$ after appearance developed detonation. The behavior of product B was the same as all reaction were taken into account like in the conceded above case (Fig. 3 and Fig. 4). Only some molecules of reagent A placed up to the hot wall because of absent of reaction $A+B\rightarrow B+B$.

So, only birth of detonation in conceded cases is connected with reaction $A+B\rightarrow B+B$ which taken place in condition of translational nonequilibrium. Spreading of detonation causes reaction $A+A\rightarrow B+A$.

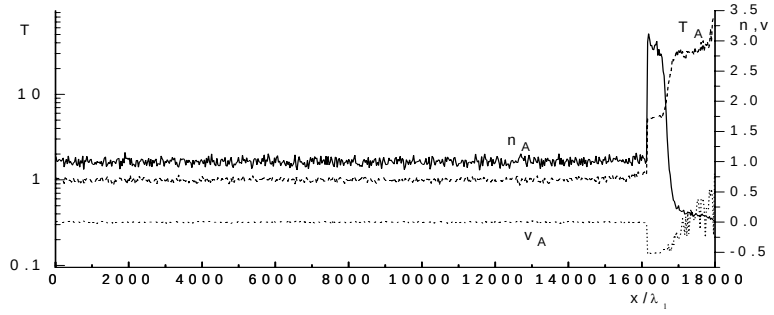

Fig. 5.

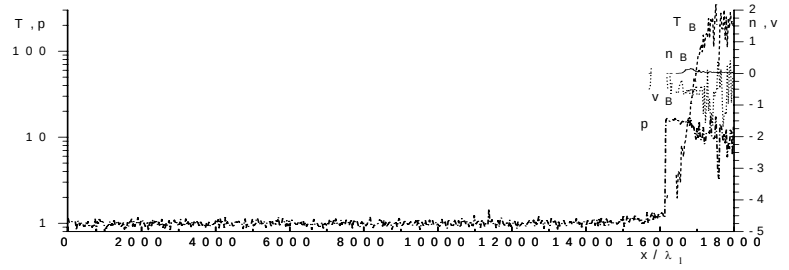

Fig. 6.

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