MULTI-PROCESSOR STATISTICAL SIMULATION OF FORMING A DETONATION WAVE IN THE SHOCK TUBE FOR CASES OF DIFFERENT THRESHOLDS OF A REACTION

S.V. Kulikov, O.N. Ternovaia

Institute of Problems of Chemical Physics RAS, 142432, Chernogolovka, Moscow reg., Russia. E-mail: kuls@icp.ac.ru

The Monte Carlo non-stationary method of statistical simulation (MCNMSS) (another name DSMC) was used in calculations. Non-stationary case of forming a detonation wave in the shock tube was considered. It was supposed that chemical reaction $A+M \rightarrow B+M$ (M=A,B and C) took place. The ratio of molecular masses of gases A, B and C was:20:20:1. Different thresholds of the reaction were considered. The cases of weak (low-pressure) detonation were obtained.

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 all processes of heat-mass transfer automatically. Development of computers permits now to simulate by MCNMSS a gas processes in which a local mean free path of molecules (l) is much less than a local character size of this process (L) except a small region where $l \sim L$. Detonation in the shock tube is one of such processes. Numerical study of process of forming a detonation wave in the gas on the molecular process level gives a lot of useful information.

2 STATEMENT OF PROBLEM

Non-stationary case of forming a detonation wave in the shock tube was considered. Simulation was carried out in the one-dimensional coordinate space and in the three-dimensional velocity space. At an initial moment, the low-pressure channel (LPC) of the shock tube was filled up of gas A. And the high-pressure chamber (HPC) was filled up of gas C. Cross-sections of HPC and LPC and initial temperatures of gases A and C were the same. At the beginning of the simulation the ratio of pressures in HPC and in LPC was equal to 100. The simulation started after removing a diaphragm between these parts of the shock tube. It was supposed that chemical reaction $A+M \rightarrow B+M$ (M=A,B and C) took place. The same reaction was considered by Anderson and his coworkers [3,4]. The ratio of molecular masses (m_i) of gases A, B and C was:20:20:1. This is analogue to the case of internal molecular energy release. The considered thresholds of the reaction (Q_{AB}) were equal to $25kT_1$, $35kT_1$, $70kT_1$, $95kT_1$ and 150 kT_1 (k is the Boltzmann constant, T_1 is the temperature in LPC and HPC at the initial moment of time). 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 walls at boundaries of the simulation region.

3 METHOD OF SIMULATION

Used method (MCNMSS) employs weight factors [1,2 (see scheme 2)]. In order to the size of spatial cell (Dx) did not exceed l in the gas, the value of spatial cell in HPC was 20 times smaller than the value of that in LPC at the beginning. During the simulation, that part LPC where molecules from HPC have enter, got new cells the value of which was 20 times smaller than the value of old sells. The initial average number of model particles per cell (N) was equal to 360 both in LPC and in HPC, initial Dx =0.15 in LPC. Here and bellow distance is normalized to mean free path in LPC at the initial moment (l_H). The time of splitting of collision and displacement stages was Δt=0.04. Here and bellow time is normalized to the ratio l_H/u, where u is the most probable thermal velocity of molecules of component C at the beginning.

Parallel calculations were carried out by means of a multi-processor computer [5]. Domain decomposition s of a simulation region was performed. Standard Message Passage Interface (MPI) [6] was used to communicate data between processors. And 200 processors were used. The modeled region spread from 0 to 5631.75 Boundary between LPC and HPC was placed at x=4882.5.

4 RESULTS

In considered case mass of reagent m_A is equal to mass of product m_B. 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 $z=2Q/kT_1$ then 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. Here and bellow velocities are normalized to u.

More interesting results were obtained when the thresholds of the reaction was equal to 150 kT_1. And they will be discussed bellow mainly. Results of simulation with lower thresholds are similar to some extent. The difference will be discussed.

Fig. 1, 2 show the results of simulation at the moment 180.2. There is no a detonation wave. Fig.1 shows profiles of macroparameters of reagent *A*: concentration (solid line), kinetic temperature (dash line) and longitudinal velocity (dot line). But, you see in this figure appearance of a shock wave. Its velocity was equal to 0.94. This velocity corresponds to Max number M=4.6. Ignition of gas *A* didn't take place. So, there wasn't product *B*. Fig.2 shows the results for gas *C* placed in the high pressure chamber initially. You can see also the profile of total pressure of gas mixture (dash and dot line). Here and bellow n, T and p are normalized to their initial values in LPC.

It should be noted that a period of reaction induction was very shot for the cases of lower thresholds of the reaction. And a shock front didn't form before forming a detonation wave for these cases.

Burning of gas *A* and forming a detonation wave took place already approximately at the moment of time 221.5 in vicinity of x=4475 (Fig. 3, 4, 5). In Fig 3, 4 one can see profiles of macroparameters of reagent *A* and product *B*. Here and bellow notations are as in Fig.1. It should be noted that the shock wave was absorbed by detonation wave quickly and was absent in Fig.3. Fig 5 shows the profile of total pressure of gas and the results for gas *C*.

Fig. 6, 7, 8 show the results of simulation at the moment 464.45. One can see a development of detonation process (Fig. 4). Forming a quasi-stationary region of the flow inside product *B* takes place. The profile of velocity shows it clearly.

Fig. 9, 10, 11 show the results of simulation at the moment 670.25. As one can see, the quasi-stationary region becomes longer. The behavior of velocity of the product *B* isn't simple. Parameters of the flow remains constant in quasi-stationary region and have these meaning: $n_2/n_1 \approx 1.25$, $p_2/p_1 \approx 360$ $T_2/T_1 \approx 280$. These values are approximately in 20%, 30% and 20% respectively less than for the Chapman-Jouguet condition. Range of variation of detonation velocity D is from 6.07 to 6.18. Mean value is equal to 6.13. It is equal approximately to Chapman-Jouguet velocity, a little higher. This is the case of weak (low-pressure) detonation. Other considered cases of simulation give also weak detonation.

CONCLUSION

The presented results show possibilities of using our method for modeling of detonation wave. There is no serious problem to consider more complex cases with several components and reactions.

The present study was supported by the Program of Presidium of RAS "Mathematical modeling and intellectual systems" (program of Presidium of RAS No 16).

REFERENCES

[1] *Genich, A.P., Kulikov, S.V., Manelis, G.B., Chereshnev, S.L.* Sov. Tech. Rev. B. Therm. Phys.. 1992. V.4. Part 1. P. 1-69.

[2] *Kulikov S.V., Serikov V.V.* 1993 Rus J Comput Mechan.. No 3. P.49—69.

[3] *Anderson, J.B., Long, L.N.* Jour. Chem. Phys. 2003. V.118. No 7. P.3102-3110.

[4} O'*Conner P.D., Long L.N., Anderson J.B*, 24rd International Symposium (M. Capitalli, Eds) Am. Inst. Phys., P.517-522).

[5] *Kulikov, S.V.,Ternovaia 0.N.,* Vichis. Metodi i Progr. 2004. V.5. No 2. P5-9. (In Russian).
[6] *Snir, M., Otto, S., Huss-Lederman, S., Walker, D., Dongarra, J.* MPI: The Complete Reference Vol. 1, The MPI Core, MIT Press, Boston, 1998.

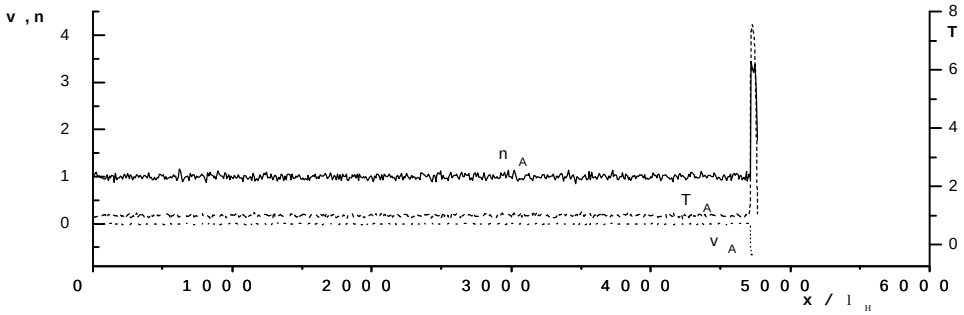

Fig. 1.

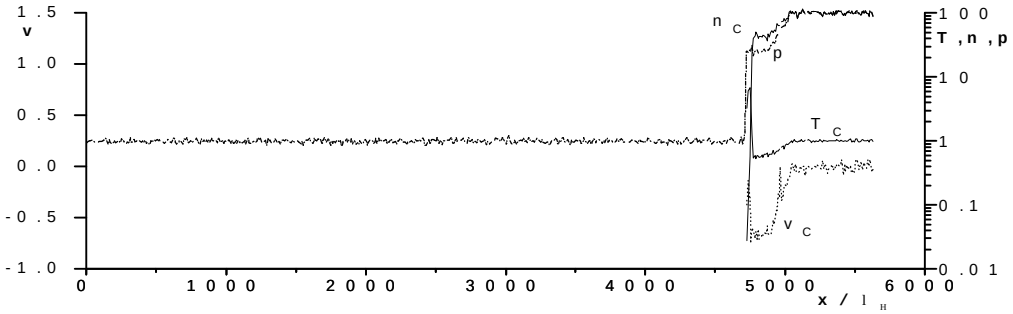

Fig. 2.

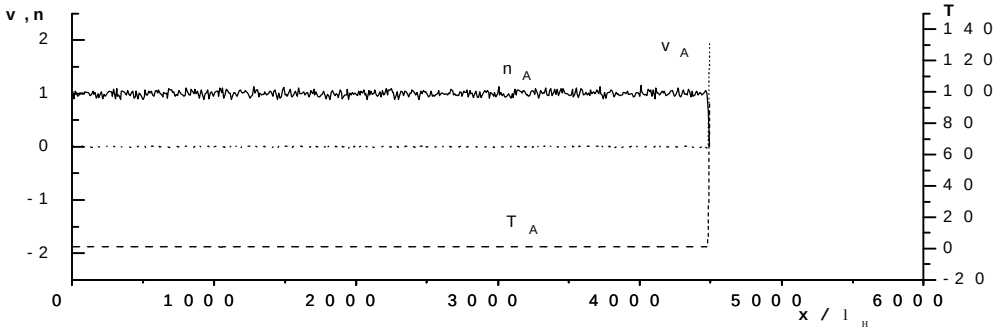

Fig. 3.

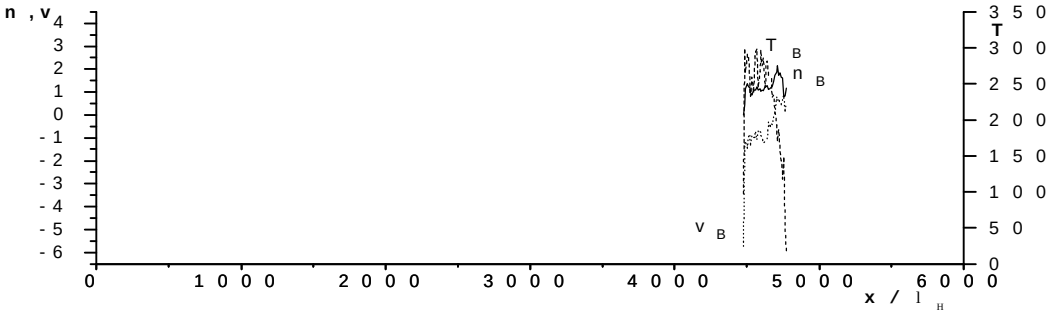

Fig. 4.

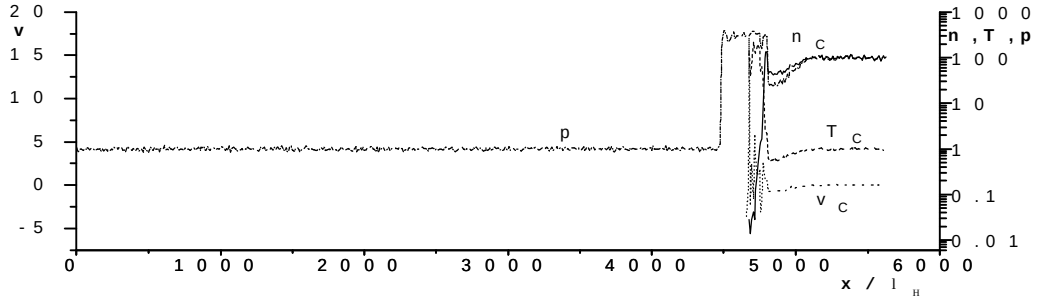

Fig. 5.

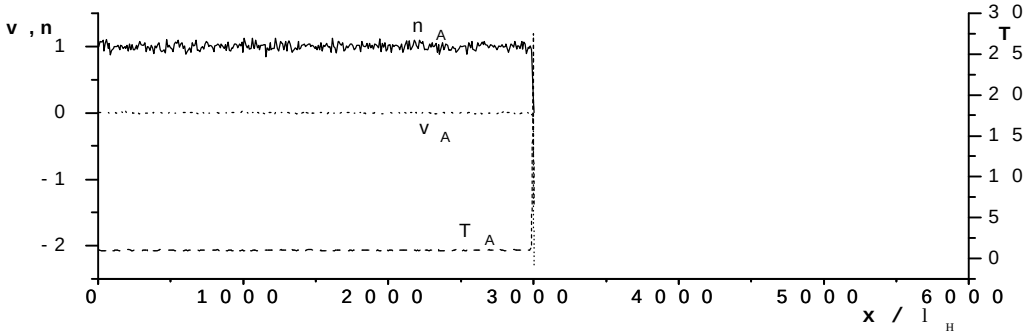

Fig. 6.

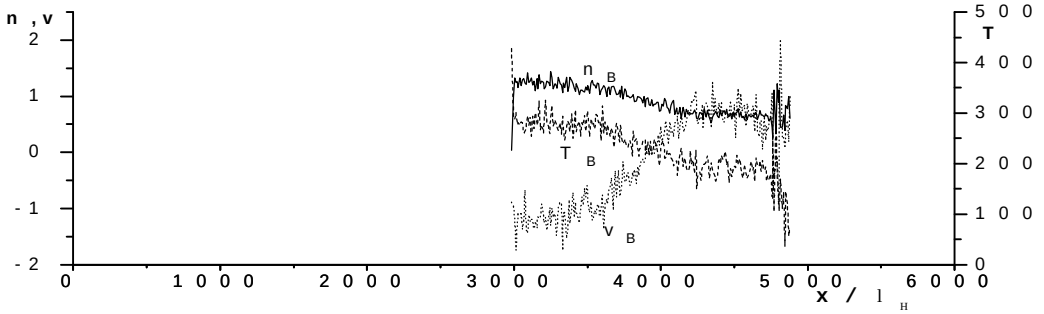

Fig. 7.

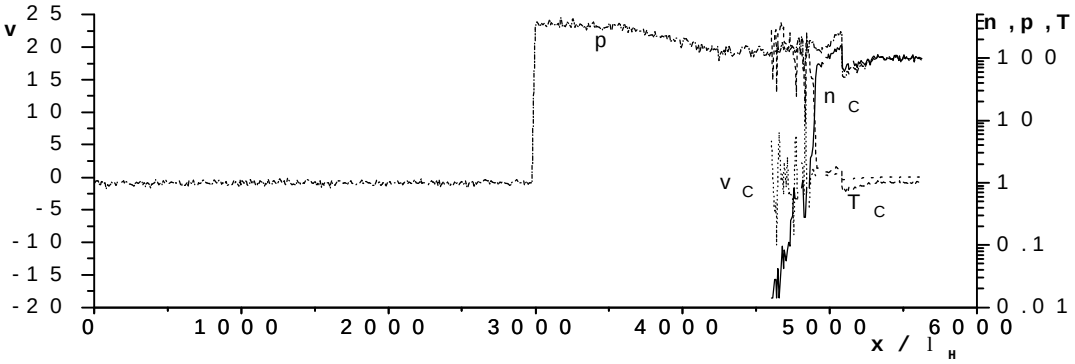

Fig. 8.

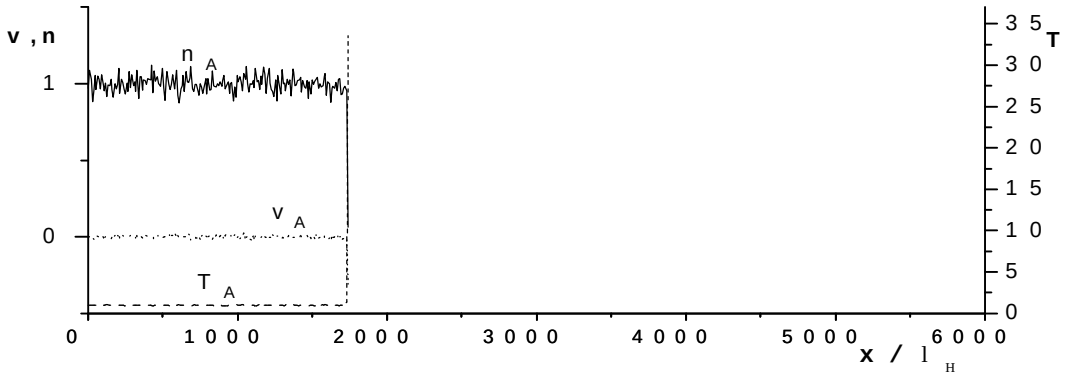

Fig. 9.

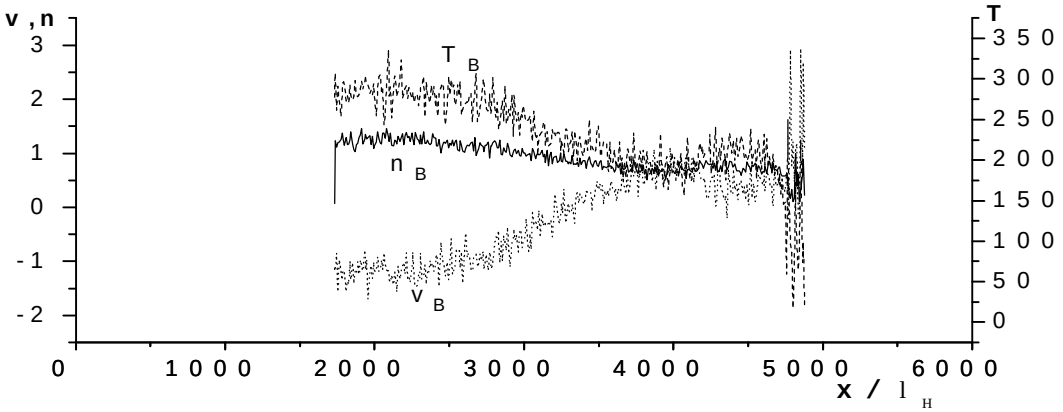

Fig. 10.

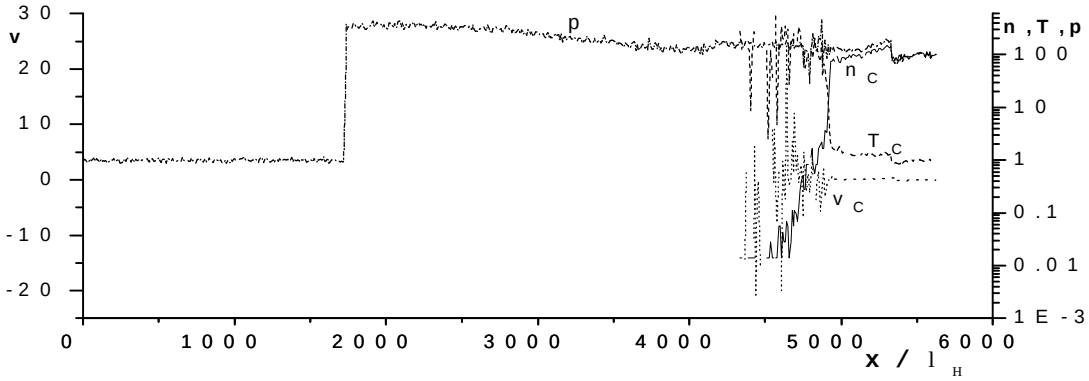

Fig. 11.