Possibility of Physical Detonation in the Flow of Vibrationally Pre-excited Hydrogen in a Shock Tube

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Abstract. The direct simulation Monte Carlo method was used to numerically simulate processes in the shock wave front in vibrationally excited hydrogen flowing in the shock tube. The cases of partially and completely excited hydrogen were considered. Equilibrium hydrogen was applied as a pusher gas, but its concentration was 50 times higher than the hydrogen concentration in the low-pressure channel. In addition, the strength of the shock wave was varied by heating the pusher gas. Number of employed processor was equal to 274. The modeling domain was split into 274 subdomains, in each of which the evolution of the system was simulated with a single processor. The parameters of the wave in the case of physical detonation become dependent on the vibrational-to-thermal energy conversion and independent of the way of its initiation. This served as a criterion for the appearance of the physical detonation in the numerical experiment. It turned out that this phenomenon occurs until the degree of pre-excited hydrogen is not less than 85% in the low pressure channel. And the vibrational temperature is not less than 2800K.

Keywords Supercomputer · Simulation · Blok decomposition · Vibrational excitation · Shock tube

1 Introduction

The detonation of gas mixtures is an interesting and complex phenomenon that has been systematically studied for more than a century [1]. The question arises as to whether physical, rather than chemical, energy concentrated on internal degrees of freedom of, say, vibrationally excited molecules may cause detonation under certain conditions. If so, this detonation can be called physical detonation [2]. Vibrationally preexcited hydrogen is the most appropriate gas for checking the feasibility of physical detonation [3].

Gas detonation and flow in a shock tube are very special gasdynamic processes. Parameters of the flow change drastically in a very narrow zone with the local characteristic size, L, comparable with the local mean free molecular path, λ, i.e. λ □ L. At the same time the local mean free molecular path is much less than the local characteristic size of other parts of the flow. However, the processes that take place in the narrow zone influence the whole flowfield. And they should be considered at the molecular level. Generally speaking, in other parts of the flow one can restrict consideration by the hydrodynamic approach, but the problem of "cross_linking" different solution methods appears in this case. Of course, it is more correct to use a method that makes it possible to consider all problems at the molecular level. At the modern state of computation techniques, this can be made by the Monte Carlo non-stationary method of statistical simulation, also known as direct simulation Monte Carlo (DSMC). The idea of the method was proposed by Bird [4]. The method gives a result without solving the Boltzmann equation and automatically takes into account all details of mass and heat transfer.

Conditions of realization of the physical detonation in a shock tube have been numerically obtained in [5]. It has been shown that the phenomenon took place in a fully vibrationally preexcited hydrogen placed in the low-pressure channel (LPC) of a shock tube. The cases of completely and partially excited hydrogen were considered. The initial vibrational temperature (T_V) was equal to 3000K. It has been shown in [5] that, if the prestored vibrational energy is weakly converted to translational energy, the shock wave slows down over time. If the energy conversion is sufficiently intense, when the pusher gas is warm and only completely vibrationally excited hydrogen is in the low-pressure channel, the wave gains velocity over time (its velocity increases roughly by a factor of 1.5). This causes physical detonation, in which case the parameters of the wave become dependent on the vibrational-to-thermal energy conversion and independent of the way of its initiation. The latter has been shown in [5] by heating the hydrogen in the high-pressure chamber (HPC) to different temperatures (T_H) (439 and 585 K) that resulted in waves of varying intensity.

Below we present results which complement the results of work [5]. Namely, cases of partially preexcited hydrogen and of lower temperatures of vibrational preexcitation were considered.

2 Statement of the problem

At the beginning, the LPC of a shock tube is filled with two portions of hydrogen. The first portion is vibrationally preexcited hydrogen The rotational and translational temperatures were assumed to be equal to room temperature T_1 = 292 K. The second portion consisted of totally equilibrium hydrogen with T_1. In other words, it was assumed that only part the hydrogen was excited (for example, by electrical discharge). A HPC was initially filled with hydrogen as pusher gas at a much higher pressure. The strength of the shock wave (SV) was varied by heating the pusher gas. Then the numerical simulation of the process in the shock tube started.

3 Simulation technique

Simulation was performed in a 1D coordinate space and a 3D velocity space using DSMC method. The basics of shock and detonation wave simulation in a shock tube with taking into account rotational and vibrational degrees of freedom of molecules were presented elsewhere [6, 7, 8]. Below, we cite the simulation algorithm for the reader's convenience.

A real medium (a medium to be simulated) was replaced by a set of model particles. According to initial conditions, the particles at zero time have the given velocities and are distributed over cells into which the coordinate space is split. It is assumed that particle collisions are binary and may occur between the particles occupying the same cell with a certain probability.

The evolution of the system over time interval Δt is divided into two stages: (i) the movement of particles with constant velocities (stage *A*) and (ii) variation of the particle velocities due to collisions. (stage *B*).

The *i*th model particle of species *l* denoted by $A_l^{(i)}$ was characterized by mass m_l, velocity $\mathbf{c}_l^{(i)}$ ($u_l^{(i)}$, $v_l^{(i)}$, $w_l^{(i)}$) coordinate in the flow $x_l^{(i)}$, and weighting factor η_l. This weighting factor indicates the number of actual molecules represented by the given model particle. Thus, the concentration of actual molecules in the *j*th cell of volume V_j is defined as

$$n_l^{(j)}=\Sigma\ h_l/V_j$$

Simulation of stage *A* is very simple. As a result of this simulation, the new position of model particle $A_l^{(i)}$ in the flow is given by

$$x_l^{(i)*}=x_l^{(i)}+u_l^{(i)}\Delta t.$$

The impact parameter used here is the integrated cross section s_{lm}^{ik} of elastic scattering between molecules $A_l^{(i)}$ and $A_m^{(k)}$. Molecules were considered as a perfectly rigid spheres.

We will henceforth use the following notation:

$$J_{lm}=\max\{h_l,h_m\},\qquad q_{lm}=\min\{h_l,h_m\}.$$

Here and below, the indices of numbers of particles and cells will be omitted for simplicity whenever possible.

At stage *B*, the evolution of the system was simulated in several (*k*) steps. At each of these steps, the interaction of pairs of particles in the cell under investigation occurred during time period $\Delta t_* = \Delta t/k$. Simulation of each such step was performed in accordance with the ballot box scheme of testing. To this end, all pairs of particles in a cell were divided into aggregates characterized by species of particles forming the pairs (e.g., pairs of particles of species 1, pairs of particles of species 1 and 2, and so on). In each aggregate, only one pair of particles (e.g., A_l and A_m) is chosen equiprobably. The evolution of the state of the chosen pair of particles was simulated in accordance with the scheme described below.

Step 1. The interaction of particles A_l and A_m was simulated with probability

$$Q_{lm}=K_{lm}\ J_{lm}\ s_{lm}g_{lm}\ \Delta t_*/V$$

Here, K_{lm} is the number of pairs of particles in the aggregate under investigation. Number *k* was chosen so that Q_{lm} was slightly less than unity. If the result of the test is negative, the next step for the given pair of particles was not made.

Step 2. Velocities of particles A_l and A_m were replaced by velocities after the collision $\mathbf{c}_l^*$ and $\mathbf{c}_m^*$ with probabilities θ_{lm}/η_l and θ_{jm}/η_m, respectively. This is the so called improved ballot box scheme of tests for simulating the collision stage.

This method was used to numerically simulate the problem of the shock wave front in vibrationally excited hydrogen flowing in the shock tube. The cases of completely and partially excited hydrogen were considered. It was supposed that unexcited H_2 was in full thermodynamic equilibrium. In the simulation, the rotational and vibrational degrees of freedom of molecules were taken into account in the simplest terms [5, 7, 8]. An energy sink model (see Section 11.3 in [4]) was employed. It should be emphasized that Monte Carlo (statistical) simulation considers the kinetic temperature as the mean energy associated with the respective degrees of freedom of a molecule. In the case of equilibrium over degrees of freedom, this temperature is the thermodynamic temperature. Each time, at the beginning of the collision stage, the total (over all translational degrees of freedom) kinetic translational temperature (T) was determined for the given type of molecules in the cell. Then, at each collision adopted, the difference Δ_i between temperature T and the temperature of a given inner degree of freedom was determined. Parameters R_{ij} were set (i - is the component number, and j = 1 or 2 for rotational and vibrational degrees of freedom, respectively). Then the internal temperature (and the corresponding internal energy) changed in the product $R_{ij}\Delta_i$ in the direction of approximation to T. When the equilibrium internal energy was determined, it was assumed that the specific heat of a molecule for the rotational and vibrational energies equals k (k is the Boltzmann constant; in units used in the simulation, $k = 0.5$) and $R_{i1} = 0.01$. However, R_{i2} depended on relative velocity g of colliding particles. At $g < 3.726$ m/s, $R_{i2} = 0$; at $3.726 \leq g \leq 9749$ m/s, $R_{i2} = 0.00005$; and, at $g \geq 9748$ m/s, $R_{i2} = 0.01$. The parameters of this model were selected so as to provide real values of vibrational relaxation time for H_2 at different temperature. When the post-collision velocities of a pair of particles were determined, it was assumed that the change in the translational energy of this par of particles is equal in magnitude and opposite in sigh to the change in the internal energy of these particles. It should be noted that vibrational degrees of freedom of H_2 are not excited when 292K. Therefore, the initial vibrational temperature and energy of the unexcited hydrogen in the LPC were supposed equal to zero.

Equilibrium hydrogen was applied as a pusher gas in HPC, but its concentration was 50 times higher than the hydrogen concentration in the LPC.

For linear size Δx of a spatial cell to be shorter than free path λ of molecules in a gas, the modeling domain in the HPC was first split into cells 20 times smaller than those in the LPC. In the process of evolution of the system, size Δx in that part of the LPC to which the gas is delivered from the HPC was also decreased by 20 times.

In addition, the strength of the shock wave was varied by heating the pusher gas in HPC. Velocity D can be increased by raising the pressure drop between the HPC and LPC. This can be done by increasing the concentration of molecules in the HPC. In this case, however, Δx in the HPC decreases further. Correspondingly, the counting time increases and the number of processors exceeds a reasonable value. A more simpler and more effective way is to raise the gas temperature in the HPC (with the number of processors remaining the same) and upgrade the computational program to a minor extent. The counting time will be change slightly. However, it should be noted that, if D is too high, the temperature in the post shock flow may also rise to excess and the change of vibrational energy will become minor again.

With the aim of using a reasonable number of model particles, the weight factor for all particles of H_2 in the HPC was taken to be equal to 5 and that for excited particles of H_2 in the LPC to 1. The weight factor for of the equilibrium unexcited hydrogen in the LPC (η_{uH}) was determined from the equation:

$$\eta_{uH} = 1/\alpha - 1.$$

Here, α is the fraction of vibrationally excited hydrogen in the LPC.

The value of Δt was set equal to 0.04. Henceforth, t is normalized to λ_1/u, where $\lambda_1 – \lambda$ in the LPC at zero time and $u = (2kT/m)^{0.5}$ is the most probable thermal velocity of the particles in the gas medium ahead of the SW (m is the molecular mass of hydrogen). The distance is normalized to λ_1. In the LPC, initially, $\Delta x = 0.15$. The linear dimensions of the HPC and LPC were 4795.2 and 10873.2, respectively. The boundary between LPC and HPC was placed at the point $x = 0$. At the beginning, the average number of model particles of each sort in the cell equaled 90.

Particles are elastically reflected from the boundaries of the modeling domain.

A multiprocessor computer MBC100K installed in the Joint Supercomputer Center of RAS was used. Its peak performance is equal to 227.94 Teraflops. The supercomputer consists of 1275 computing module (10572 cores).

The block decomposition of the modeling domain was applied [6, 7]. The modeling domain was split into 274 sub-domains, in each of which the evolution of the system was simulated with a single processor (core). After each step of movements, information about particles that leave sub-domains occupied by them at the beginning of the given step and pass to neighboring sub-domains was transferred to the latter sub-domains using the SEND and RECV procedures from the MPI library [9]. Thus, by increasing the number of processors up to several thousand, one can extend the modeling domain virtually without increasing the counting time (at a fixed time of the system's evolution), since data exchange takes place between neighboring sub-domains. The transfer time for this information is almost independent of the number of processors. Experience has shown [6, 7] that this organization of parallel computation is the most reasonable.

4 Results of the simulation

First, the simulations were carried out for cases when the fractions of vibrationally preexcited hydrogen were equal to 0.85 and 0.75 at the vibrational temperature of 3000K. It was shown that only the initial excitation of 85% H_2 led to the physical detonation. And it was absent for lesser degree of excitation. An increase in wave velocity with time had occurred for $\alpha = 0.85$ at T_H 584, 657 and 730K (see Fig. 1)

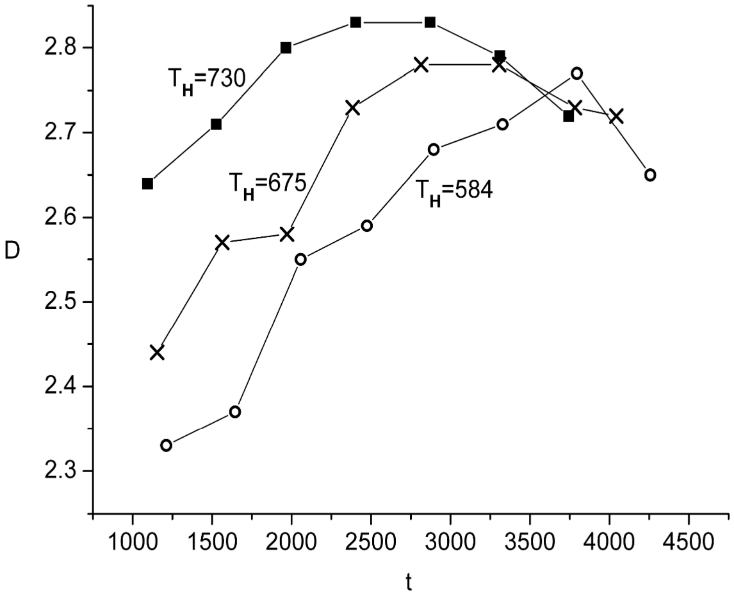

Fig. 1. Wave velocity *D* vs. simulation time *t* for $T_V = 3000$ at different T_H, α =0.85.

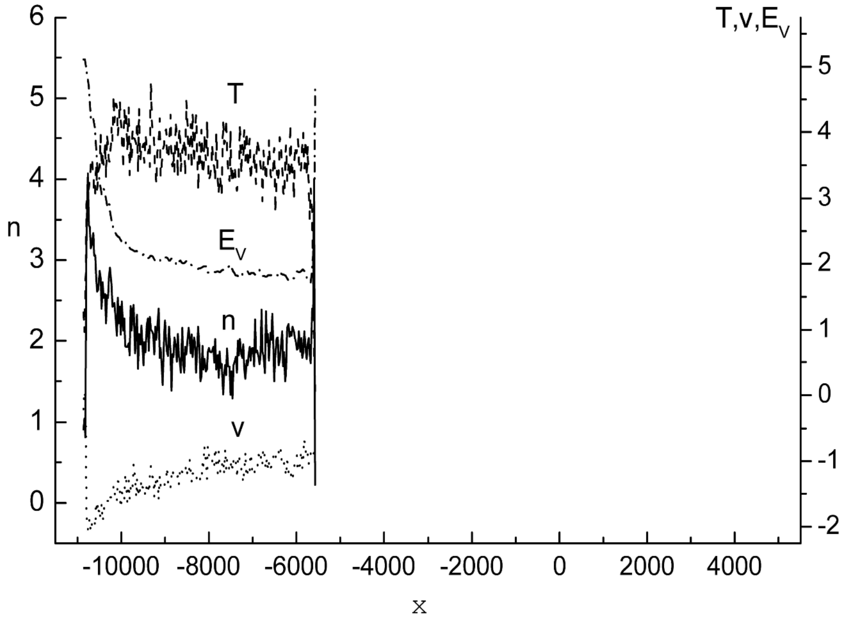

Fig. 2. Profiles of concentration (*n*), temperature (*T*), velocity of the flow (*v*) and internal vibrational energy of initially excited H_2 (E_V), T_H = 584K.

Henceforth, D is normalized to u. The accuracy of determining of D values was within ±0.05.

Fig. 2 and 3 demonstrate simulation results obtained for the case when the HPC was initially filled with completely equilibrium hydrogen heated to T_H = 584K, α = 0.85. Simulation time t was equal to 4257.775. This time corresponds to the moment when the front came very close to the left end of the simulation region. Profiles of parameters in the post-shock flow (a region of a shock-heated gas in the LPC) are shown in Fig. 2 for vibrationally preexcited H_2. Fig. 3 demonstrate profiles of parameters of initially completely equilibrium hydrogen. Henceforth, concentration n is normalized to initial concentration of vibrationally preexcited H_2 in the LPC. Total kinetic translational temperature T is normalized to T_1. Velocity of the flow v is normalized to u. Normalized energy E_V is given by equation

$$E_V = k(T_V/T_1),$$

where T_V is the running vibrational temperature. The dimensionless initial vibrational energy E_V of the hydrogen equaled 5.14 for initial T_V = 3000K. It is necessary to remind that k is the Boltzmann constant. In units used in the simulation, k is equal to 0.5.

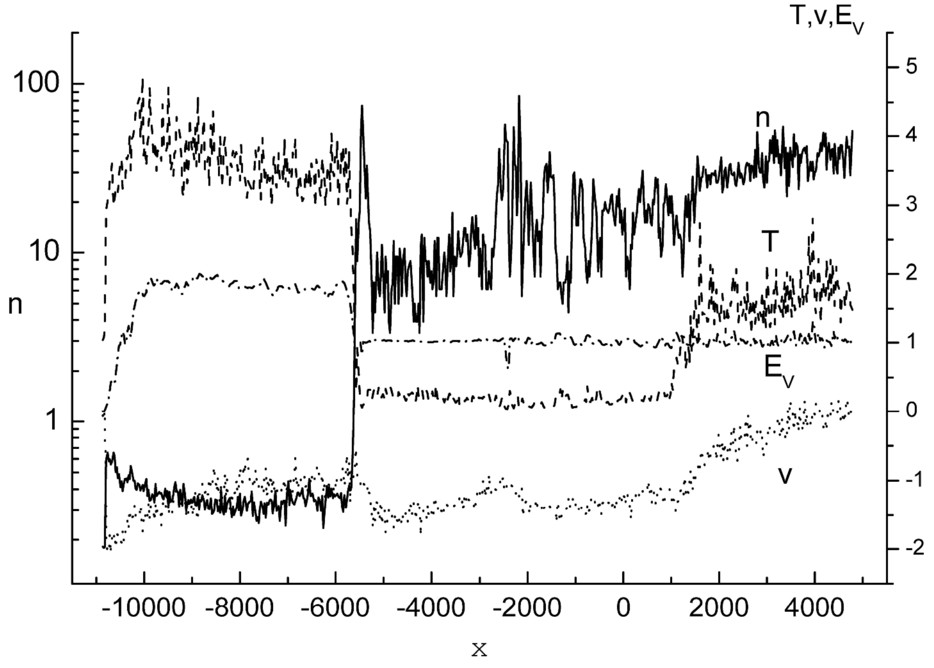

Fig. 3. Profiles of n, T, v and E_V of initially equilibrium H_2, T_H = 584K.

Fig. 4 and 5 show results obtained for the case when the HPC was initially filled with completely equilibrium hydrogen heated to T_H = 730K, α = 0.85. Simulation time t was equal to 3742.85. This time corresponds to the moment when the front came very close to the left end of region of the simulation. As above, profiles of parameters in the post-shock flow are presented in Fig. 4 for vibrationally preexcited H_2. Fig. 5 demonstrates profiles of parameters of initially completely equilibrium hydrogen.

Fig. 3-5 illustrate the flow picture when high wave velocity was already installed. The profiles of flow parameters in the post-shock flow coincide with each other with accuracy of statistical dispersion at T_H 584 and 730, despite the varying intensity of the initial shock waves. The profiles of parameters obtained at T_H 675K give that kind of same picture. And they are not shown in the article. All these results convincingly testifie to the achievement of the physical detonation.

Next, simulations were carried out for initial excitation of 85% H_2 to the vibrational temperatures 2900 and 2800K. Fig. 6 and 7 demonstrate the growth of wave velocities over simulation time and achievement their stationary values. Fig. 6 shows the dependence of wave velocity on the simulation time at T_H 584 and 675K for T_V =2900K.

These results and the corresponding profiles of flow parameters in the post shock flow at high D (for example at t more 4000) testifies to the achievement of the physical detonation. The correspondent profiles at T_H 584 and 657K are very similar to each other as above (see Fig, 3-6). They are not given in the article due to lack of space.

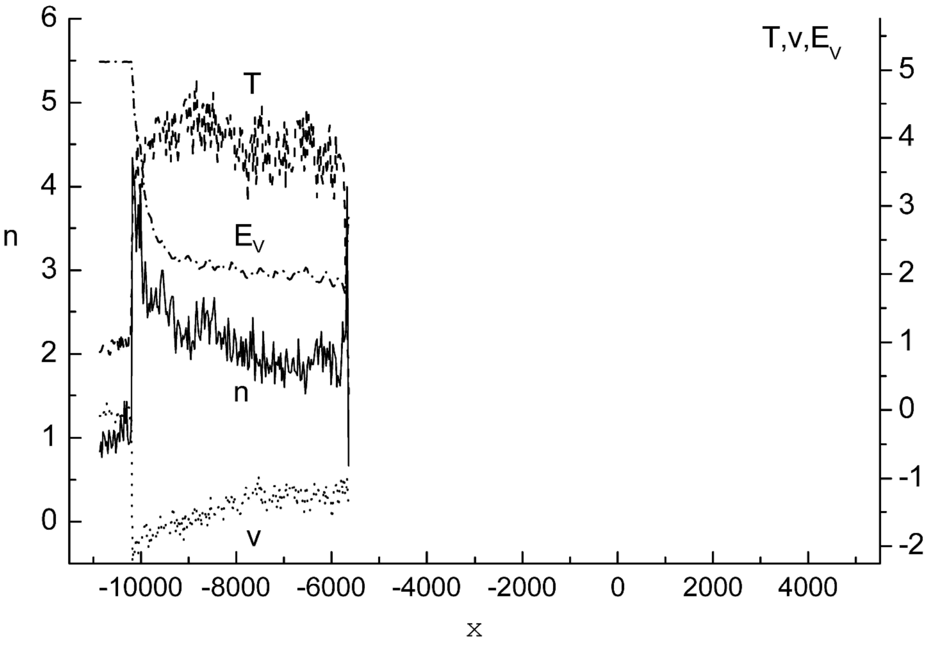

Fig. 4. Profiles of n, T, v and E_V of initially excited H_2, T_H = 730K.

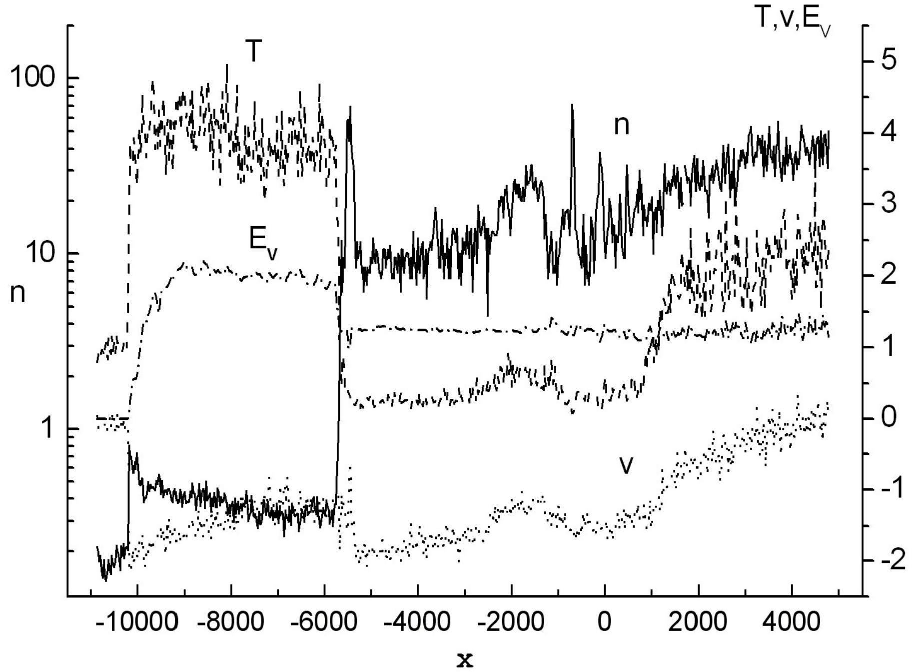

Fig. 5. Profiles of n, T, v and E_V of initially equilibrium H_2, T_H = 730K.

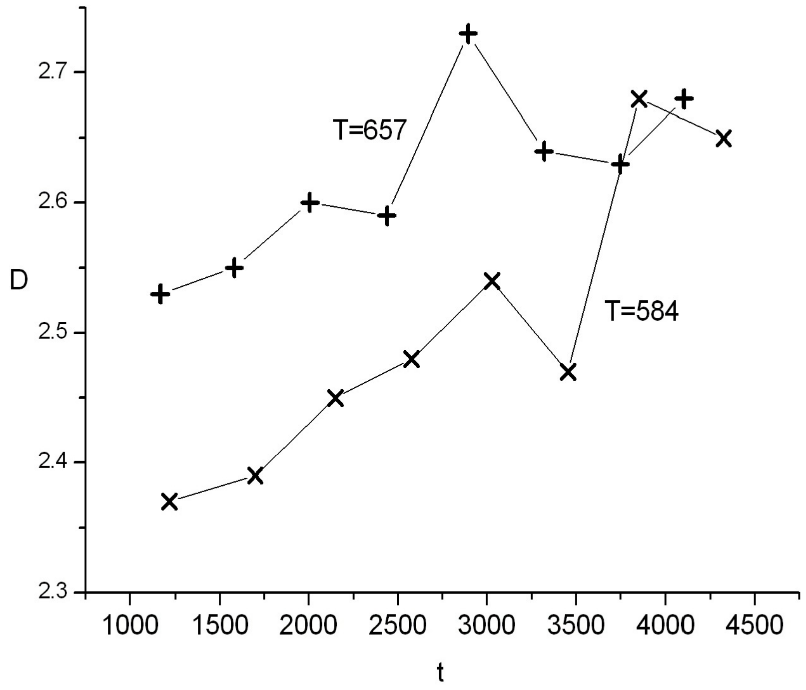

Fig. 6. Wave velocity D vs. simulation time t for T_V = 2900K at different T_H, α =0.85.

Fig. 7 shows the dependence of wave velocity on the simulation time at T_H 657 and 730K for T_V =2800K.

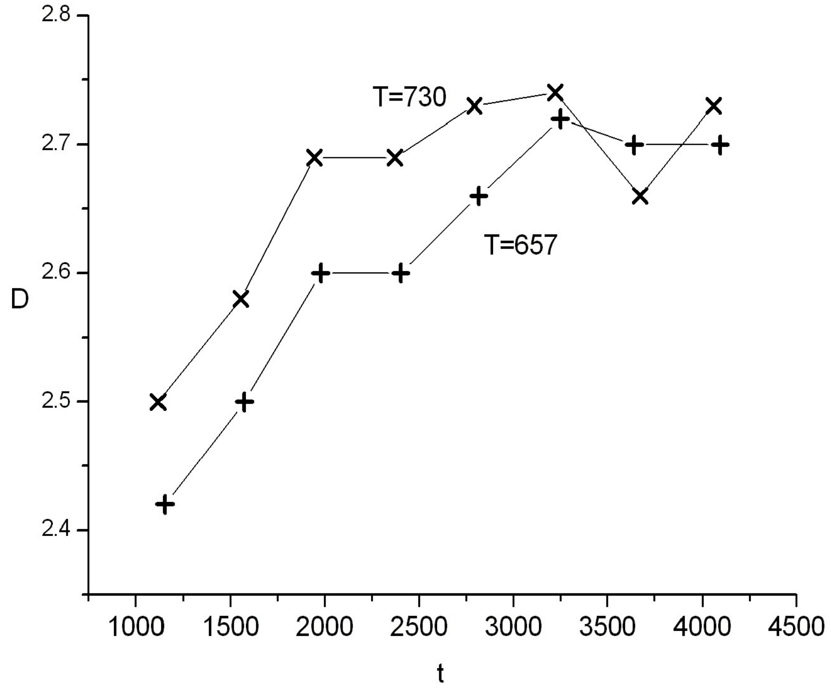

Fig. 7. Wave velocity D vs. simulation time t for T_V = 2800K at different T_H, α =0.85.

Fig. 8 and 9 show results obtained for the case of T_V 2800K when the HPC was initially filled with completely equilibrium hydrogen heated to $T_H = 730$K, $\alpha = 0.85$. Simulation time t was equal to 4095.425. This time corresponds to the moment when the front came very close to the left end of region of the simulation. Profiles of parameters in the post-shock flow are presented in Fig. 8 for vibrationally preexcited H_2.

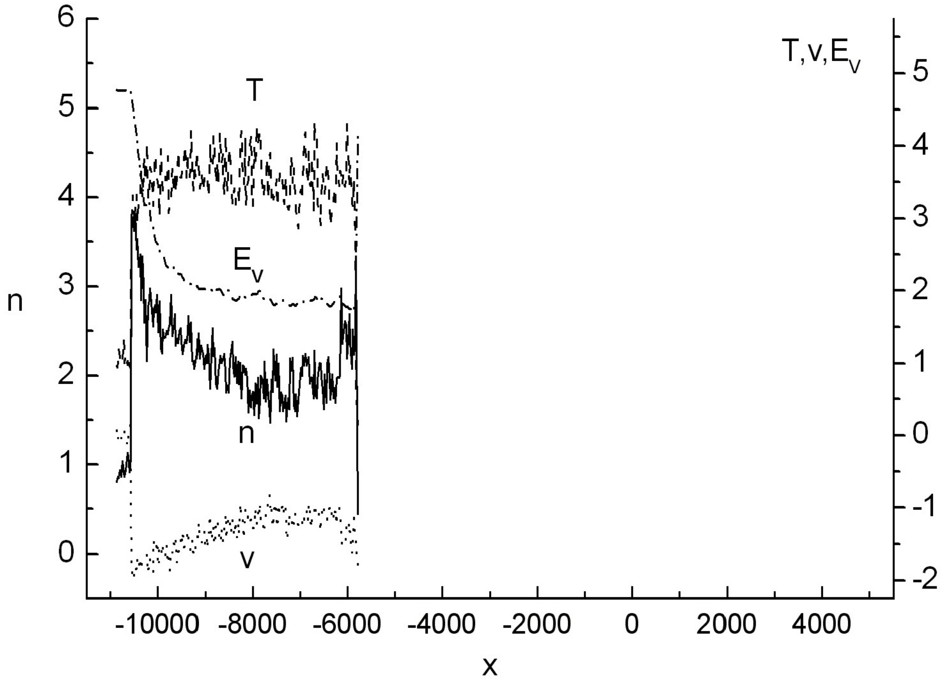

Fig. 8. Profiles of n, T, v and E_V of initially excited H_2 for $T_V = 2800$K, $T_H = 657$K.

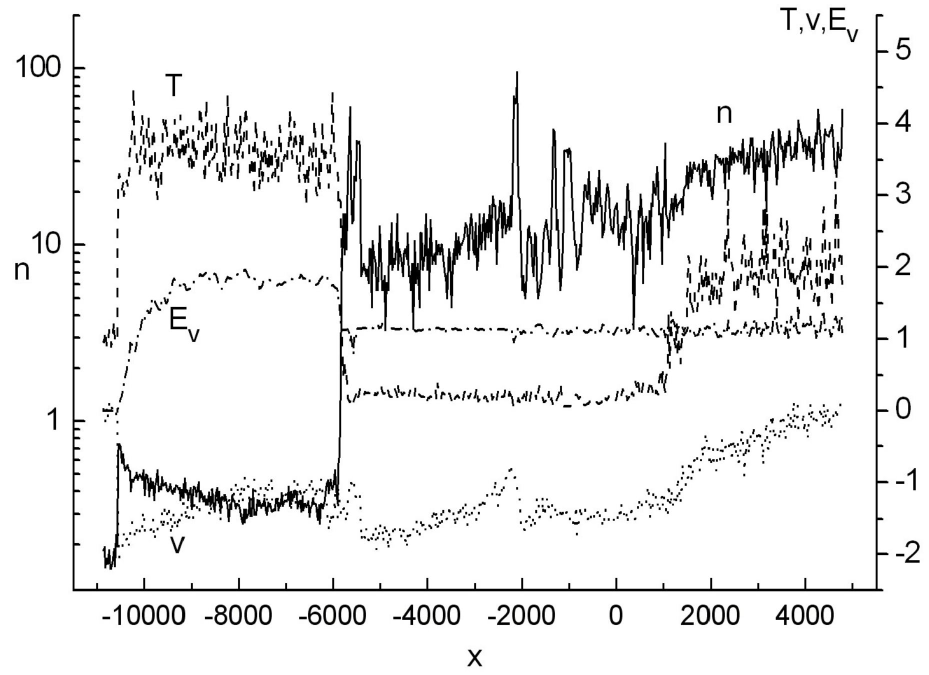

Fig. 9. Profiles of n, T, v and E_V of initially equilibrium H_2 for $T_V = 2800$K, $T_H = 657$K

Fig. 9 demonstrates profiles of parameters of initially completely equilibrium hydrogen.

Fig. 10 and 11 show results obtained for the case when the HPC was initially filled with completely equilibrium hydrogen heated to T_H = 730K, α = 0.85. Simulation time *t* was equal to 4058.875. This time corresponds to the moment when the front came very close to the left end of region of the simulation. Profiles of parameters in the post-shock flow are presented in Fig. 10 for vibrationally preexcited H_2.

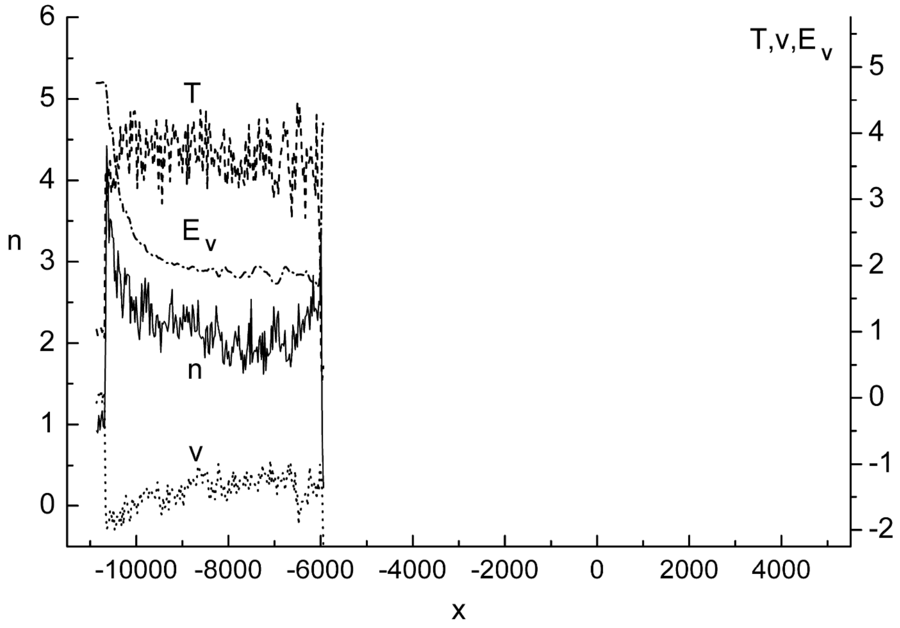

Fig. 10. Profiles of *n*, *T*, *v* and E_V of initially excited H_2 for T_V = 2800K, T_H = 730K.

Fig. 11 demonstrates profiles of parameters of initially completely equilibrium hydrogen.

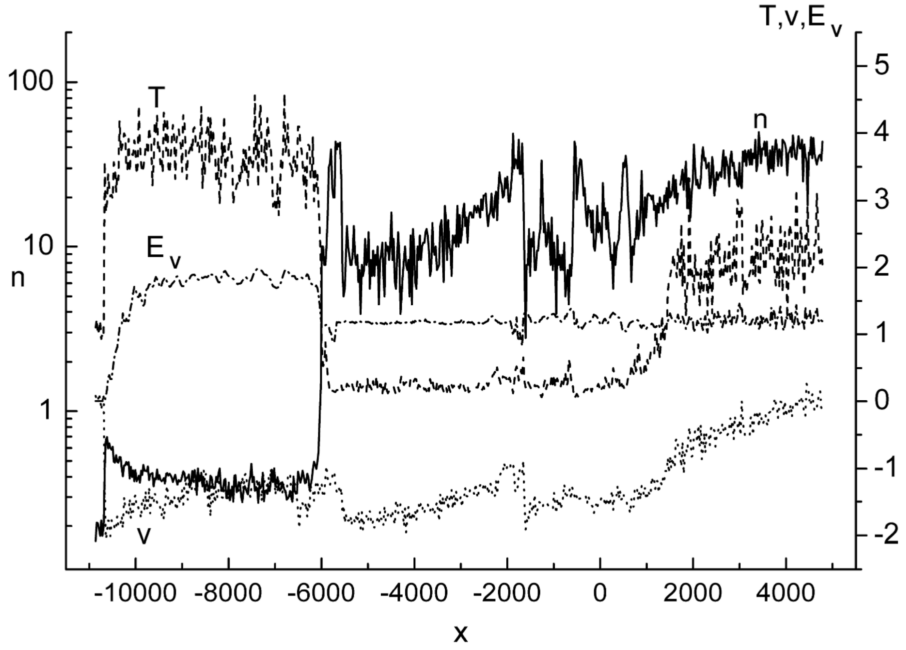

Fig. 11. Profiles of *n*, *T*, *v* and E_V of initially equilibrium H_2 for T_V = 2800K, T_H = 730K.

Fig. 8-11 illustrate the flow picture when high wave velocity was already installed. The profiles of flow parameters in the post-shock flow coincide with each other with accuracy of statistical dispersion at T_H 657 and 730, despite the varying intensity of the initial shock waves. All these results convincingly testifie the achievement of the physical detonation.

The profiles of parameters obtained at T_V 2900K give that kind of same picture. And they are not shown in the article.

The normalized initial vibrational energy of hydrogen is consistent with 4.97 and 4.79 for the initial vibrational temperature 2800 and 2900K. This information is presented for the reader's convenience.

4 Conclusions

A powerful computational program was created for the supercomputer. Simulation of the flow of hydrogen in a shock tube was performed. The cases of the vibrationally preexcited hydrogen were considered. The number of used processors (cores) was equal to 274.

It was shown numerically that the physical detonation may take place at milder conditions compared with the predicted in [5]. It turned out that this phenomenon occurs until the degree of preexcited hydrogen is not less than 85% in the low pressure channel. And the vibrational temperature is not less than 2800K.

The simulation results obtained for a wider region of parameters confirmed the conclusions given in the paper [5]. Indeed, as for a classical detonation wave, the parameters of the physical detonation wave are independent of the way of detonation initiation. When the shock wave evolves to a physical detonation wave, its velocity markedly grows.

The obtained results can be useful for researchers in their experimental realization of the physics detonation.

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