Numerical Simulation of H_2/O_2 Continuous Spin Detonation with a Detailed Chemical Mechanism

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1 Introduction

Very high energy release rates, which can be achieved in detonations, for many years attract attention of engineers to possible practical applications of this phenomenon. As was shown for the first time by Ya. B. Zel'dovich [1], the detonation regime of combustion is also more efficient thermodynamically than the deflagration under the same initial conditions. One can hope that development of detonation-based fuel-burning devices will eventually lead to the design of more cost-effective and compact engines for of sub-orbital spacecraft and other high-speed vehicles. In recent years, significant efforts were undertaken for a detailed research on the concept of Pulse Detonation Engine (PDE), a device which creates propulsion by burning the fuel in a combustion chamber where a traveling detonation wave is periodically initiated. Nevertheless, it seems that, owing to the difficulties of fast exhaust of the combustion products and recharging of the combustion chamber by the fresh fuel mixture, the current generation PDEs are not yet capable of running at high frequencies needed for efficiency.

There are a few alternative concepts of detonation-based engines. In particular, a promising idea that can be traced back to the work of B. V. Voitsekhovskii [2] is to use a detonation wave spinning in an annular tube, which is constantly refilled by a combustible mixture from one end. It is the so-called Continuous Detonation Wave Engine (CDWE), which was mostly studied in the Lavrent'yev Instutute of Hydrodynamics, Novosibirsk, Russia. In many aspects, CDWE is close to PDE operating at very high frequency (several kHz). For a review of this concept and its comparison with PDE, see the recent publications [3,4].

In the present work, the detonation wave propagation in CDWE is simulated numerically by solving the Euler equations for a chemically reacting flow. A detailed chemical model (6 species, 7 reactions) is used to describe the combustion of stoichiometric hydrogen-oxygen mixture. The governing equations are solved with a high-resolution shock-capturing WENO (weighted essentially non-oscillatory) scheme. The numerical simulations are used to obtain a clear picture of processes in the combustion chamber of CDWE, elucidate the underlying physical mechanisms, and investigate the influence of different parameters on this phenomenon.

2 Problem formulation, governing equations and numerical method

A typical combustion chamber of CDWE is an annular cylindrical tube with one closed and another open ends. The mixture of fuel and oxidizer is injected from the closed end through a ring slit or a number of regularly arranged small holes. Depending on the conditions of initiation, the detonation wave travels azimuthally in the

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clockwise or counter-clockwise direction. It burns the layer of combustible gas, which is restored to the time when the following wave arrives. The combustion products flow towards the open end and then discharge from the chamber through a diverging nozzle. Due to heat release, the supersonic flow velocity can be achieved though the device has no geometrical throat.

It should be noted that the numerical simulation of CDWE in the full 3D configuration can be too expensive for a parametric study. The problem can be simplified by assuming that the gap between the tube walls is small in comparison with its radius and the flow variations in the radial direction are negligible. This approximation is used in the present paper so that the computations are performed in a 2D rectangular domain with the periodical boundary conditions imposed along one coordinate direction. The size of the computational domain along x (the periodicity length) is denoted thereafter as l whereas its length along y is L. The stoichiometric mixture of H_2 and O_2 is injected through the lower boundary at $y = 0$. The injection conditions are determined by the mixture total pressure P_{tj} and temperature T_{tj} (300 K in all computations), the net area of slit or holes divided by the whole area of the closed end wall A_j, and the maximum injection flow rate $G_{j\max}$. The actual mass flow rate depends on the wall pressure distribution $P_w(x)$. It is assumed that the injection is performed through a system of nozzles so that the local injection mass flow rate is zero for $P_w \geq P_{tj}$ and equal to $G_{j\max}$ for $P_w \leq P_{crj}$, where P_{crj} is the pressure at which the sonic injection condition is achieved. The fluxes of conservative variables due to injection are added to numerical fluxes calculated by the flow solver in the first row of grid cells next to the wall. It is assumed that, starting from $y = L_1$, the tube cross-section linearly increases with y, which is simulated by introducing geometrical source terms into the governing equations. This tube expansion results in a supersonic flow velocity on the whole outflow boundary so that simple extrapolation boundary conditions can be utilized there.

The Euler equations for the mixture of thermically perfect gases are solved. The standard (CHEMKIN) polynomial dependencies of enthalpy on temperature are used for all species. The ONERA chemical mechanism which was developed for supersonic combustion computations (see, e.g. [5]) is adopted here to calculate the chemical source terms. It includes six species, H_2, O_2, H_2O, H, O, and OH and 7 chemical reactions. Preliminarily, the model has been validated by comparing the ignition delay time and reaction time for the conditions corresponding to the detonation wave propagation with the results obtained from more detailed chemical mechanisms.

The computational code is based on the shock-capturing WENO scheme of the fifth order [6]. In contrast with more wide-spread TVD schemes, the WENO ones do not decrease their accuracy down to the first order near smooth extrema of the solution. Thus, they add to the solution a significantly smaller amount of numerical diffusion and allow one to resolve the flowfield much better. The WENO scheme is used here along with the semi-implicit additive Runge-Kutta scheme ASIRK2C [7] for time integration. It enables us to avoid the severe time step restrictions resulted from the stiff chemical terms and advance the solution in time with a constant CFL number. The code is parallelized using the MPI library. Usually, 10 processors are used for the computations presented below. The flow solver has previously been validated by computing 1D ZND detonations and 2D cellular detonation waves.

3 Results of computations

First, numerical simulations have been performed for the combustion chamber with $l = 100$ mm and $L = 120$ mm that approximately corresponds to the optimal parameters of the perspective rocket CDWE considered in [3]. The length of constant area tube is $L_1 = 100$ mm while the remaining part expands linearly so that the final cross-section area increases twofold. The computational grid consists of 1000×470 cells; it is uniform along x with the increment $\Delta x = 0.1$ mm. The minimum step size in the y direction is also $\Delta y = 0.1$

mm but, starting from $y = 25$ mm, the grid along y is gradually stretched. At the initial moment, the chamber is filled by the combustion products except a triangular region of the fresh mixture, which is placed by the tube closed end.

After the detonation initiation, a complicated transient process takes places and then the flow approaches to a periodical regime. A typical instantaneous flowfield observed during the periodical stage is shown in Fig.1.

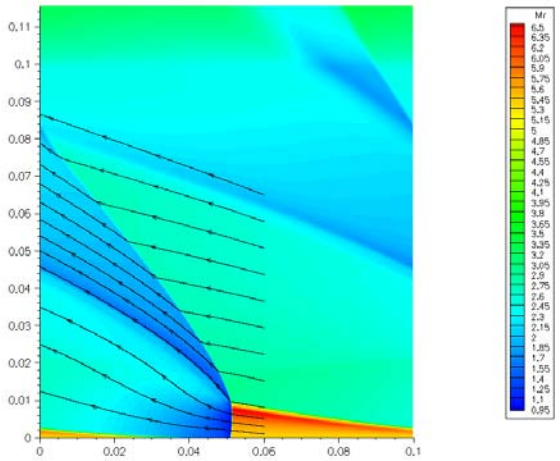

Fig.1. Streamlines and Mach number flowfield calculated in the detonation wave frame of reference.

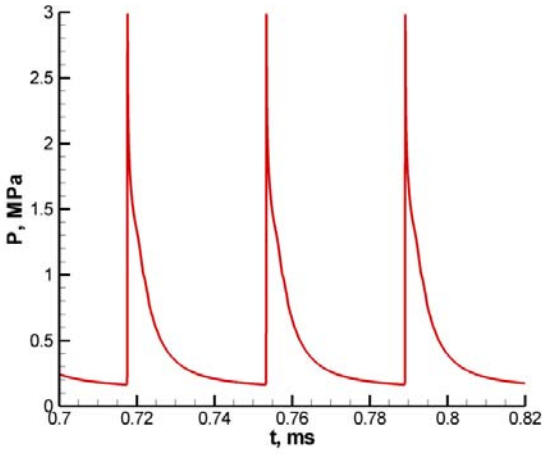

Fig.2. Pressure history in some point on the wall during three periods of rotation.

Here the injection parameters are $P_{tj} = 1$ MPa and $A_j = 0.133$. At these conditions, the maximum mass flow rate is $G_{j\max} = 200$ kg/(s·m^2), however, since the high pressure values behind the detonation wave suppress the injection for some time, the actual value of the mean mass flow rate is smaller. When the periodical regime is established it is equal to $G_j = 172.45 \pm 0.075$ kg/(s·m^2). It should be noted that, in the first computations, we encountered an unexpected phenomenon: due to numerical diffusion the ignition occurred not only behind the detonation wave but also on the contact boundary between the fresh mixture and the combustion products. The velocity of this "pseudolaminar" flame was about 10 m/s and usually 10-20% of mixture was burnt by that flame. To avoid this problem, the chemical source terms on the contact boundary were artificially suppressed. With this modification, the difference between the injected mass and that burnt in the detonation wave does not exceed 0.1%.

The general flow structure is clearly visible in Fig. 1. The propagating detonation wave burns the layer of fresh mixture injected from the lower boundary and separated from the combustion products by a contact discontinuity. Under the present conditions the maximum height of the combustible layer h is 9.5 mm. The injection is suppressed just behind the detonation wave. There is also a shock wave in the combustion products, which is attached to the detonation wave in the triple point where the latter meets the contact discontinuity. The third wave, an expansion fan, is emanated from the triple point behind the detonation front. The fan turns the stream upwards aligning it with the deflected contact line. All these structures closely resemble experimental pictures of the spin detonation in [4].

The pressure history in some point on the wall in the periodic regime is given in Fig.2. A strong regularity of pressure variations is evident. The time averaged maximum peak pressure is $P_{w\max} = 2.985 \pm 0.003$ MPa, the minimum pressure $P_{w\min} = 0.165$ MPa, the mean wall pressure $\overline{P}_w = 0.446$ MPa. The time period between the successive pressure peaks is $\tau = 35.79 \pm 0.004$ μs. It corresponds to the detonation wave velocity $D' = 2794$ m/s in the laboratory frame of reference. Taking take into account the flow velocity ahead of the detonation wave,

one obtains the detonation wave velocity $D = 2829$ m/s with respect to fluid. It is slightly less than the Chapman-Jouguet velocity $D_{CJ} = 2864$ m/s calculated with the EQUIL code from the CHEMKIN II library at the initial pressure $P_\infty = 0.116$ MPa and temperature $T_\infty = 281$ K.

Numerical simulations have also been performed for a shorter combustion chamber with $L = 60$ mm and the length of the constant area section $L_1 = 40$ mm. The wall pressure distributions and mean flow rates obtained for two different geometries have been virtually identical. Also, more refined grid in the y direction with the minimum increment $\Delta y = 0.05$ mm has been used to investigate the grid independence of the solution obtained. The comparison has shown that the numerical flowfields do not change significantly so that the present resolution can be considered as adequate.

The dependence of main flow characteristics on geometrical extensions of chamber, the injection pressure, and the relative injection area has been studied. All these results will be presented in detail during the conference.

4 Conclusion

Numerical simulations of continuous spin detonation in the stoichiometric hydrogen/oxygen mixture have been performed using a detailed chemical mechanism and a shock-capturing scheme of a high order. The periodic regime of detonation wave propagation has been reproduced and studied. High resolution numerical flowfields in the combustion chamber of perspective CDWE have been obtained and time averaged values of flow parameters have been evaluated. The numerical flowfields demonstrate the flow structure, which has been observed in experimental works, and allow one to elucidate major features of the investigated phenomenon. A parametric investigation has also been conducted using different chamber sizes and injection conditions.

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