Numerical simulation of detonation on the basis of Harten scheme

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The mathematical model corresponding simplified model of two-phase chemical reaction, including the induction period and the subsequent reaction period was used for numerical simulation of detonation in gas mixes oxygen-hydrogen. Gas was assumed ideal and non viscous. Two problems have been calculated: cycle of the pulse detonation engine and a spontaneous detonation of an air-hydrogen mix under a protective environment of a nuclear reactor.

1 Introduction

The system of the equations of ideal gas and the kinetic equations in the integral form for axial symmetric flows can be presented [1,2] as follows:

$$\frac{d}{dt}\oint_V \overrightarrow{Q}dV + \oint_S \overrightarrow{n}FdS + \Phi = 0; \tag{1}$$

$$\overrightarrow{Q} = (\rho, \overrightarrow{m}, \rho e, \rho b, \rho\alpha); F = (\overrightarrow{m}, (\overrightarrow{m}\overrightarrow{m})/\rho + PI, \overrightarrow{m}(e+P)/\rho, (\overrightarrow{m}\overrightarrow{B})), \overrightarrow{B} = (\beta, \alpha),$$

$$\Phi = (0,0,0,0,\rho w_\beta, \rho w_\alpha), P = \rho RT, e = RT/(\gamma-1) + \overrightarrow{V^2}/2 + \beta q,$$

$$w_\alpha = \frac{d\alpha}{dt} = \frac{-1}{\tau_{ind}} = -k_1 P\exp(-E_1/RT),$$

$$w_\beta = \frac{\beta}{dt} = -k_2 P^2\beta^2\exp(\frac{-E_2}{RT} - (1-\beta)^2\exp(-\frac{E_2+q}{RT}),$$

where $\rho, P, e, \overrightarrow{m}, T, R$ density, pressure, energy, impulse vector, temperature and gas constant, accordingly. Parameters α, β characterize promotion of reaction: during induction period $\beta = 1, 0 \le \alpha \le 1$, during reaction period $\alpha = 0, 0 \le \beta \le 1$, for oxygen-hydrogen mixes $\gamma = 1.4$, q - heat effect of chemical reaction, k_1, k_2, E_1, E_2 - coefficients of reaction.

2 Numerical method

Surface integral in (1) for control volume in the form of spatial six lateral wedge (in axial symmetric coordinates - the quadrangle) can be presented as follows:

$$\oint_S \overrightarrow{n}FdS = \sum_{j=1}^{4} T^{-1}\overrightarrow{H}\overrightarrow{S_j} + \overrightarrow{S_k}\overrightarrow{E};$$

where $\overline{H} = (\rho u, \rho u^2 + P, \rho v u, \rho u + P u, \rho\beta u, \rho\alpha u)^T$, $E = P(0,0,1,0,0,0)^T$, S_k - area of lateral side of cell boundary, T - matrix of transition from axial symmetric to curvilinear coordinates , $\overrightarrow{n} = (n_x, n_y)$, $\overrightarrow{\tau} = (\tau_x, \tau_y)$ - normal and tangential vectors to the side of cell S_j, $u = \overrightarrow{n}\overrightarrow{V}, v = \overrightarrow{\tau}\overrightarrow{V}$. Flow vector on the side of cell calculated by the formulae:

$$H = (H_l + H_r + \sum_{j=1}^{6} \widetilde{\alpha}_j |\widetilde{\lambda}_j| \widetilde{e_j})/2,$$

where $\widetilde{a_j}, \widetilde{e_j}$ – eigen values and right eigen vectors of matrix $\partial\overrightarrow{H}/\partial\overrightarrow{Q}$, calculated on the side of cell with using Roe's averaged gas dynamics variables [3]. Vector $\overrightarrow{\alpha} = L\Delta\overrightarrow{Q}$ - product of dependent unknowns vector of sistem (1) in delta-form with left eigen vectors matrix; $\widetilde{\alpha}_j$ – components of vector $\overrightarrow{\alpha}$. The numerical algorithm is developed on the basis of finite volume method with using the TVD scheme [4] of second order of accuracy is used for numerical approximation of system of the equations (1). The operator of a time step – difference approximation of system (1) is split on symmetric sequence of step operators in directions [5]:

$$U^{n+2} = L(2\Delta t)U^n;\ L(2\Delta t) = L_i(\Delta t)L_j(\Delta t)L_j(\Delta t)L_i(\Delta t)$$

$$L_i(\Delta t) = I - \frac{\Delta t}{V_i}[\hat{F}_{i+1/2}\overrightarrow{S}_{i+1/2} - \hat{F}_{i-1/2}\overrightarrow{S}_{i-1/2} + \overrightarrow{S_k}\overrightarrow{E}]$$

$$\hat{F}_{1/2} = 1/2[\hat{F}_0 + \hat{F}_1 + \hat{R}_{1/2}\hat{\Phi}^{\alpha}_{1/2}] \tag{2}$$

Let's design components $\hat{\Phi}^{\alpha}_{1/2}$ as $(\Phi^{\alpha}_{1/2})^k$, then:

$$(\ \Phi^{\alpha}_{1/2})^k = 1/2\Psi(a^k_{1/2})(g^k_0 + g^k_1) - |a^k_{1/2} + \gamma^k_{1/2}|\alpha^k_{1/2}, g^k_i = (1 + \omega^k\theta^k_i)\ limiter(\alpha^k_{i+1/2}, \alpha^k_{i-1/2}),$$

$$\gamma^k_{1/2} = \begin{cases} 1/2\Psi(a^k_{1/2})(g^k_1 - g^k_0)/\alpha^k_{1/2}, \alpha^k_{1/2} \neq 0 \\ 0,\ \alpha^k_{1/2} = 0. \end{cases}$$

$$\Psi(z) = |z| - \lambda z^2, \alpha^k_{1/2} = \overrightarrow{L}^k_{1/2}(\overrightarrow{U}_1 - \overrightarrow{U}_0), \theta^k_0 = |\alpha^k_{1/2} - \alpha^k_{-1/2}|/(|\alpha^k_{1/2}| + |\alpha^k_{-1/2}|),$$

where $\omega^k \in [0,2]$ – – the parameters of artificial compression. The parameter λ determines the accuracy of scheme for time variable. The limiters were used of two types, namely, Harten's [4]and Roe's [2] (Superbee). Calculation grids were generated on Thompson type algorithm [6], based on decision of sistem of Poisson equations, description of procedure in details was made in [5].

3 Calculation results

Transition to dimensionless variables has been made, values of scale factors where choose according to [2]. After transition to dimensionless variables value of constants in (1) where accepted, corresponding the mixture composition hydrogen-oxygen-nitrogen - 20, 10, and-70 percent, accordingly: $q = 20, E_1 = 1.7, E_2 = E_1/4.9, K_1 = 3.6, K_2 = K_1/20$.

3.1 The calculation of pulsing detonation engine cycle

The flow, corresponding to the cycle of the pulsing detonation engine [7,8], was calculated. The scheme of the engine is taken from [8]. The gas mix containing combustible component (hydrogen or acetylene) moves to the resonator through ring nozzle in the form of a ring supersonic jet. The pulse detonation engine itself consist of the resonator of hemisphere form on which the fuel mix in the form of a ring supersonic jet acts. Idea of authors [8] is that leaving ring nozzle the supersonic jet should be focused

in a vicinity of the center of the resonator, generating a shock wave extending to walls of the resonator. Reflected from walls of resonator the shock wave in turn is focused about the center of sphere, generating a detonation of an air-hydrogen mix. The arisen detonation wave which again extends to walls of the resonator, is reflected from it and forms the reflected shock wave. This wave moves to the exit of reactor on products of combustion, breaks off the jet veil, and the reacted gas mix is thrown out from a cavity of the resonator with supersonic speed, simultaneously the new cycle of engine work begins.

The calculation results demonstrated pulsing character of flow is observed, however a detonation of the gas mixture appears not in a vicinity of the center of sphere, but in vortical structures of a ring jet. It seems, that such mechanism of appearance of the detonation is more realistic for essentially non-stationary and pulsing flows then authors of [8] one of exact focusing of a shock wave in the center of the sphere.

3.2 The calculation of combustion and detonation of air-hydrogen gas mix under containment of nuclear reactor

Numerical simulation of various regimes of burning and detonation of a mix air-hydrogen under a protective environment (containment) of nuclear reactor of the atomic power station for reactors of type VVR is made. The calculation region consist of the cylinder (reactor mine), covered with a hemisphere (a dome of containment). Regimes of combustion and a detonation of hydrogen were simulated by a part of calculation region in which at the zero moment of time an instant burning of hydrogen is simulated by sudden rising of temperature and increasing of normal to border component of speed up to the values, corresponding Chapmen-Juget wave(sudden detonation).

The purpose of calculation was the estimation of peak values of pressure on walls of a containment for the forecast of its destruction. According to it the excess of value of pressure along the dome of containment during the calculation in consecutive moments of time was estimated.

4 Conclusions

The model of two-phase chemical reaction is rather rough approach and badly describes chemical structure of a detonation, however, in a combination of using the difference schemes of the high order of accuracy is quite successfully applied to simulating flows with complex structure of discontinuities [11,12] and widely enough used for simulating qualitative structure of flow. The results of calculations demonstrate working capacity of a technique for a wide range of parameters of ideal reacting gas. Resolution of used the Harten's scheme allows to observe precise structure formed detonation and shock waves and to estimate size of peak values of gas dynamics parameters.

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