Numerical Simulation of Deflagration and Initiation of Detonation

S.N.Martyushov
Committee of Energy, State Duma of Russian Federation
Moscow, Russia

T.Elperin,O.Igra
Department of Mechanical Engineering Ben Gurion University of the Negev
Beer Sheva, Israel

1 Introduction

Transition from deflagration to detonation or from shock wave to detonation one is rapid non stationary process with different scale of flow changing. In period of deflagration gas velocity is usual essential subsonic and systems of equations, simulating this process can be numerical integrated with large scale time steps. Near moment of transition to detonation system of first-order ODE's kinetic equations became stiff one and very small time step should be used.

Different mathematical models are used for simulation of detonation process: Euler or Navier -Stokes equations, including or ignoring heat-conductivity and diffusion terms for gas dynamics process, and full or simplified system of kinetic equation. As usual in numerical simulation splitting of time-step operator into gas dynamics step and kinetic step is used. In addition to physical different scale of time step of this two process sometimes algorithms of different numerical accuracy are used. Investigation of summary numerical accuracy of whole time step operator can be found, for example, [1]

2 Mathematical model

The mathematical model introduced in [2] and 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 non viscous. the system of the equations of ideal gas and the kinetic equations in the integral form for axial symmetric flows can be presented as follows:

$$d/dt\int_V \vec{Q}dV + \oint_S \vec{n}\hat{F}dS + \Phi = 0 \qquad (1)$$

Correspondence to: martyush@mail.ru

where conservative unknowns vector will be: $\vec{Q} = (\vec{U}, \vec{B}), \vec{U} = (\rho, \vec{m}, \rho e), \vec{B} = (\rho\beta, \rho\alpha)$, $\alpha = 1/\tau$ - parameter of induction, β - parameter of reactive component density, $\Phi = (0,0,0,0, \rho w_\beta, \rho w_\alpha)$ - source term, vector of fluxes normal to boundary of control volume can be written in the form:

$F = (\vec{m}, \vec{m}/\rho + PI, \vec{m}(e+p)/\rho, \vec{m}\vec{B})$

Arrhenius hypothesys is predicted for speeds of kinetics unknowns:

$$w_\alpha = \frac{d\alpha}{dt} = \frac{-1}{\tau_{ind}} = \begin{cases} -k_1 P \exp(-E_1/RT), w_\beta = 0; \\ 0, w_\beta > 0, \end{cases} \quad (2)$$

$$w_\beta = \frac{d\beta}{dt} = \begin{cases} -k_2 P^2 \{\beta^2 \exp(-E_2/RT) - (1-\beta)^2 \exp(-(E_2+q)/RT)\}, w_\alpha = 0; \\ 0, w_\alpha > 0, \end{cases}$$

where $P = \rho RT, e = RT/(\gamma - 1) + \vec{V}^2/2 + \beta q$, q - energy of reaction.

Despite of simplicity this kinetic model is widely spread because of it preserves mean features of full system of kinetic equations: Arrhenius hypothesys of functions form, period of induction instead of time period of radical component appearance and backward reaction possibility. Essential features of coefficients in Arrhenius formulae are evident for simplified system (3) and not clear for full system of kinetic equations. Non dimensioning procedure was made analogous to [3].

3 Numerical algorithm

Two types of time discretisation were used. The first method consist of splitting the explicit time step operator in symmetric consequence of operators in directions (this methods preserve 2-nd orders of time accuracy if operators in direction are 2-nd order of accuracy). The other way of time discretisation is using of explicit third order Runge-Kutta method, which gives 3-rd order accuracy for time. On the basis of both schemes explicit time step algorithm for simultaneous decision of gas dynamics and kinetic equations, described lower, was introduced. For spatial discretization vector of fluxes in the normal to the boundary direction is determined on the basis of two similar TVD - scheme, the first is the slightly improved version of the Harten scheme [4], that was suggested in [5]. and the second is Chacravarthy one [6]. For first scheme special operator of artificial compression and two types of limiter operators were used: operator minmod introduced by Harten and operator superbee, introduced by Roe. For the second scheme original limiter operator, introduced by authors, was used. Let the time step operator corresponding to (1) will be:

$$\frac{dQ_i}{dt} = L(Q_i) \quad (3)$$

Than multi step explicit Runge -Kutta operator for system (1) solution will be:

$$\vec{Q}_i^{(j)} = \sum_{k=0}^{j-1} [\alpha_{jk} \vec{Q}_i^{(k)} + \Delta t \beta_{jk} L(\vec{Q}^{(k)})], j = 1,...,m, \vec{Q}_i^{(0)} = \vec{Q}_i^n, \vec{Q}_i^{(m)} = \vec{Q}_i^{n+1}.$$

This procedure gives m -th order accuracy for time. We used Runge -Kutta scheme of third order accuracy. The numerical approximation of the time step operator (3) takes form

$$\vec{Q}_{ijk}^{n+1} = \vec{Q}_{ijk}^n - \Delta t / Vol_{ijk} \sum_{ijk} S_i \vec{F}_i^n, \vec{F}_i^n = \hat{F}_i^n \cdot \vec{n}_i \quad (4)$$

where summation is made over sides of control volume, and $\vec{F}_i^n, S_i$ are vectors of fluxes through this sides. Let explicit operator of numerical solution of ODE's system (2) (developed, for example, on the Gear's method) will be $\vec{w}^{n+1} = \vec{O}(\vec{w}^n, \vec{Q}^n, t^n, t^{n+1})$. If we will use TVD scheme of third order of

accuracy [6] for spatial approximation of fluxes $S_i \vec{F}_i^n$ in (4), full numerical explicit algorithm for simultaneous decision of gas dynamics and kinetic systems of equation can be written in the form:

$$L(\vec{Q}^{(k)}, \vec{w}^k): \ 1.\ \vec{F}_i^n = \vec{F}_i^n(\vec{U}^n, \vec{B}^n), 2.\ \vec{B}^{n+1} = L_B(\vec{B}^n, \vec{U}^n, t^n, t^{n+1}), \quad (5)$$

$$3.\ \vec{Q}_{ijk}^{n+1} = \vec{Q}' - \Delta t / Vol_{ijk} \sum_{ijk} S_i \vec{F}_i^n(\vec{Q}_{ijk}^n, \vec{w}^n), \text{where } \vec{Q}' = (\vec{U}^n, \vec{B}^{n+1}).$$

4 Grid construction

For elliptic numerical grid generation Thompson type algorithm [7], based on solving the system of three Poisson equations, was used. Curvilinear elliptic grids of this type are close to orthogonally ones and preserve property of equidistance of theirs points. That's why it needs essentially less points of grid than for Cartesian grid for the same accuracy of numerical decision. Sequence of grids with doubling number of points where used for confirming convergence of numerical decisions**.**

5 Results and discussion

Flows in channels with constrictions

For testing algorithm (5) flows in cylindrical channels with constrictions (investigated in [8],) were numerically simulated. Different type of detonation engines constructions consist of nozzles of special form, ring nozzles for example. In theoretical and numerical investigation widely used assumption that those nozzles are supersonic Laval nozzle. In reality this is not ideal Laval nozzles. Deflagration of gas mixes and transition to detonation can appear in this channels. The calculation grids (from 5000 till 50000 points) for two cylindrical channels with one and two constrictions of special form are depicted on the Fig.1.

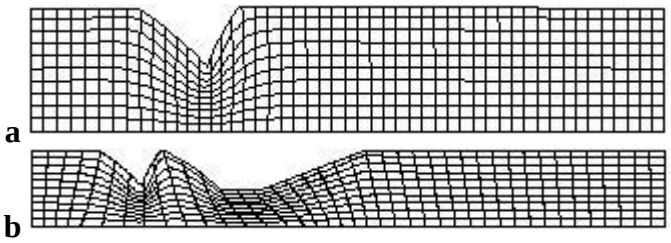

Fig.1 Calculation grids for two channels with one (a) and two (b) constrictions (every fifth line is drown).

At the initial time moment gas mix with reactive component fulfills cannels, except their left ends before the constrictions. These areas, separated by diaphragms, consist of ideal gas with high pressure and temperature ($P_1 = 26at, T_1 = 794K$ **).** At $t = 0$ diaphragms are destroyed and shock wave of high intensity propagate to the region of low pressure. Shock wave initiates high speed deflagration, which transferred to detonation wave for configuration Fig.1,b and not transferred to detonation for configuration Fig.1,a. This is depicted on Fig.2 a,b, by isopicts (light grey lines) and level lines of density reactive component of gas mix (black). Detonation wave on Fig 2,b coincide with frontal shock wave. Deflagration front on Fig.2,a is far back from front shock wave. As was shown in [8] detonation appears initially in region between constriction and strengthened in cylindrical part of small radius after second constriction. This result was repeated in present calculations.

Fig.2 Isopicts (grey) and level lines of density of reactive component (black) of flows in channels with one (a) and two (b) constrictions.

Flow in pulsing detonation engine

A pulse detonation engine is a type of propulsion system that utilizes detonation waves for efficient combustion of the fuel and oxidizer mixture. Different designs of detonation engine have been proposed and investigated during the past decades. The advantage of type of detonation engine, introduced in [9] are: the absence of moving parts in its design; continuity injection of fuel into resonator; very high frequencies of cycles. This engine comprises a reactor, where fuel-oxidizer mixture is prepared for detonation and a and resonator chamber of semi-sphere form, Fig.3,a.

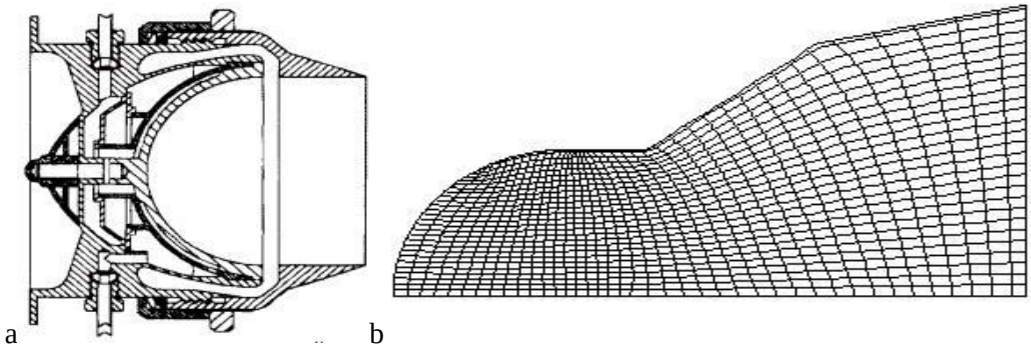

Fig.3 Scheme of Resonator of PDE with ring nozzle (a), and calculation grid (every fifth line is drown), includes semi-sphere of resonator and part of outer space of jet exit (b).

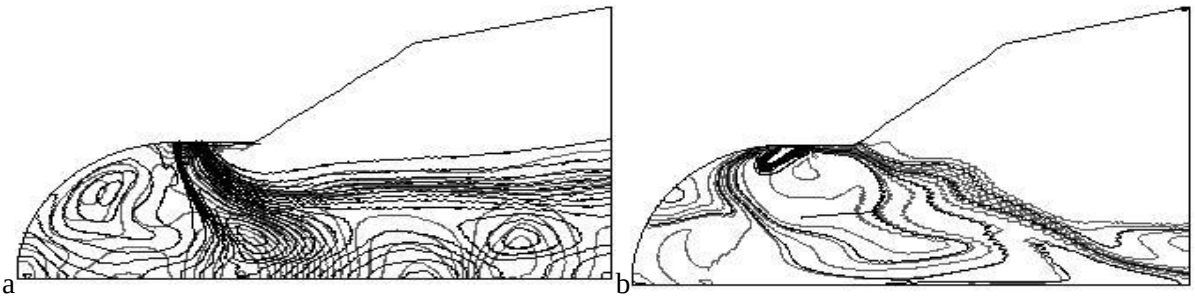

Fig.4 Isopicts (grey) and level lines of density of reactive component (black) of flows in resonator and part of outer space for $P_{exit} / P_{critical} = 0.8$ - (a) and $P_{exit} / P_{critical} = 0.08$ - (b).

Gaseous mixture flows from the reactor into the resonator through a ring nozzle. The parameters that determine the flow apart from the composition of the fuel-oxidizer mixture are the magnitudes of pressure and temperatures in the reactor and in the external space and the sizes of the exit cross-section and the critical cross-section of the ring nozzle. On the exit section of ring nozzle the gas

dynamics parameters are defined as the decision of Laval's nozzle problem. In the resulted variants of calculation the values of parameters, similar to used in [9], have been chosen: $P_r / P_0 = 3.5, T_r / T_0 = 2$; Two types of resulting flows were defined as numerical simulation results: flow with low amplitude of gas dynamic parameters frequencies for ratio of pressure in the Laval nozzle $P_{exit} / P_{critical} = 0.8$; and essential periodical one for $P_{exit} / P_{critical} = 0.08$.

The results of calculations, illustrated on Fig.4,a,b, shows up, that with using the parameters of flow, close to specified in [9], 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 near the ring jet. It seems, that such mechanism of appearance of the detonation is more realistic for essentially non-stationary and pulsing flows then one in [9], where declared the exact focusing of the shock wave in the center of the sphere.

Even in periodical flow (Fig.4,b) amplitudes of density and velocity in exit section of resonator rich their maximum values not at every time cycle. This results confirm ones of [10], where numerical simulation where made for different meanings of pressure in reactor: $P_r / P_0 = 3.5$.

6 Results and discussion

The present results of numerical simulation of flow in detonation resonator of PDE are compliment to ones of [9,10]. As was emphasized in [10] investigation with this PDE construction must be continued with different meanings of gas dynamics parameters, constructions of resonator and nozzles and realistic compounds of gas mixes

References

[1] Mahmoudi Y., Mazaheri K. (2009) Operator splitting in simulation of detonation structure. Proc.of the 22-nd of ISDERS, Minsk-2009.

[2] Levin V.A., Markov B.B. (1975) Detonation appearence during concentrative providing of energy. Russian Jorn. Phys. of Combust. and Explos. 11: 623

[3] Taki S. Fujivara T. (1978) Numerical analyses of two-dimensional non stationary detonation waves. AIAA Jornal. 16: 93.

[4] Yee H.C., Warming R.E., Harten A.(1985) Implicit Total Variation Diminishing (TVD) Schemes for Steady-State Calculation. J. Comp.Phys. 57: 327

[5] Martyushov S.N.(1996) Calculation of two non stationary problems of diffraction by explicit algorithm of second order of accuracy. Russian Jorn.Comp. Technol., Novosibirsk. 1: n.4, 82.

[6] Chakravarthy S.R., Osher S.(1985) A new class of high-accuracy TVD schemes for hyperbolic conservation laws. AIAA Paper. 85 -0363**.**

[7] Martyushov S.N.(1998) Numerical grid generation in computational field simulation. Proceedings of the 6-th International Conf. Greenwich Great Britain 249.

[8] Semenov I.V., Utkin P.S., Markov V.V. (2008) Numerical simulation of two-dimensiondetonation flows on multi-processor computers. Russian Jour. of Comput.l methods and Programming. 9: 119.

[9] Levin V.A., Nechaev Y.I., Tarasov A.I. (2001) New approach to organisation of working process of pulsing detonation engine. Russian Jorn. Chemical Phys. 20: 90.

[10] Taki S. Fujivara T. A numerical study of detonation resonator. analyses of two-dimensional non stationary. Pulse and continuous detonation propulsion. Eds. G. Roy, S. Frolov. Moscow: TORUS PRESS, 2006, p. 309