Numerical simulation of gas flows with deflagration in two-dimensional regions

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Annotation. Algorithm of two-velocity calculation is developed for two models of system kinetic equations and system of gas dynamics equations on the basis of explicit TVD schemes for flows of deflagration of hydrogen-air gas mixes. Calculations where provided for test problems of deflagration initiation from thermal spot and propagation of deflagration front in isolated cylinder and axisymmetric channels with obstacles.

Keywords: nonlinear explicit TVD schemes for multi component reactive gas mixes, branching chain reaction, detonation engine.

Introduction

Employment of hydrogen as motor fuel instead of decreasing amounts of oil and gas is treated by many authors as main way of future energetic (so called hydrogen energetic). Main preference of hydrogen as a fuel is detonation fuel cycle which is more energetic preferable in comparing with ordinary fuel cycle [1]. In connection with this preference (beyond the problems of producing, collecting and transporting of hydrogen) problem of constructing hydrogen detonation engine is extreme actual. Perspective results are projects of pulsing detonation engine [1] and spin detonation engine [2,3]. Nowadays investigations in this field are provided mainly by mathematical modelling methods. Essential part of investigations is developing and improving of mathematical methods for numerical simulation of deflagration initiation and transition from deflagration to stable detonation in hydrogen-air gas mixes flows. From the kinetic point process of transition to detonation can be treated as transition from slowly deflagration to branching chain reaction in hydrogen-air mix.This reactions where developed by N.N.Semenov [5].

Kinetic model

Equations of chemical reactions can be presented as follows:

$$\sum_{i=1}^{n} \alpha_{ij} A_i = \sum_{i=1}^{n} \beta_{ij} B_i,\ j = 1,...,M \qquad (1)$$

where *M,N* –number of reactions and components of the mix α_{ij}, β_{ij} - coefficients of direct and inverse reactions. Arrhenius low is predicted for calculating of speeds of changing of mix components concentration c_i:

$$\frac{dc_i}{dt} = \sum_{j=1}^{M} (\beta_{ij} - \alpha_{ij}) w_j(\vec{c}, T), \qquad (2)$$

$$w_j(\vec{c},T) = k_f(T)\prod_{i=1}^{n} c_i^{\alpha_{ij}} - k_b(T)\prod_{i=1}^{n} c_i^{\beta_{ij}}\,, \tag{3}$$

$$k_{f,b} = A_{f,b}T^{l_{f,b}}\exp(-E_{f,b}/RT)) \tag{4}$$

For preserving of non decreasing of entropy condition coefficients of inverse reaction where calculated from equilibrium constants:

$$k_b / k_f = K = \exp[\sum_{i=1}^{n}(\beta_{ij} - \alpha_{ij})(\frac{G_i^0(T)}{RT} + \ln\frac{RT}{P_0})], \tag{5}$$

where $G_i^0(T)$ -Gibbs potential for mix component.

For numerical solving of system (2)-(5) for hydrogen-air mix different numbers of reactions and mix components are used. In the papers of different authors ([6-8] for example) meanings of coefficients $k_{f,b}$ diverse essentially. Results of numerical simulation of flows with deflagration and detonation essentially depends of what system of reactions and meanings of coefficients $k_{f,b}$ where used. One of the aims of present work is testing of different systems of reactions and meanings of coefficients in model (2)-(5).

Gas mix of 9 component : H_2, O_2, H, O, H_2O, OH, HO_2, H_2O_2, N_2 was treated. Components as Ar, O_3 , NO, NO_2 where neglected.

For present investigation the next 9 most widespread reaction where choose:

Table 1. Chemical reactions

$-H_2+O_2=2OH$	$-H_2+OH=H+H_2O$	$-2HO_2=H_2O_2+O_2$
$-H+O_2=O+OH$	$-H_2+O=H+OH$	$-HO_2+M=H+O_2+M$
$-H_2+M=2H+M$	$H_2O_2+M=2OH+M$	$OH+H_2O=H+H_2O_2$

Characteristic feature of hydrogen-air gas mix deflagration is appearance of sudden explosion after long period of induction .In this induction period grows of radicals *H, O* and *OH* appears. Mass of radicals, nevertheless stay small, and one radical component transverse to the others.

This explosion mechanism is branching chain reaction introduced by N.N.Semenov [4].

Two sets of coefficients meanings where used for system of equations (2)-(4),for reactions from Table 1: the first from [10] (for slow deflagration simulation), the second from [5] (for calculation on the basis of branching chain reaction theory).

2. **Numerical simulation of flows of hydrogen-air reactive mixes**

The system of the equations of ideal gas and the kinetic equations in the integral form for two dimensional flows with source term which are velocities of changing gas mix components (2) can be presented as follows:

$$d/dt\int_V \vec{Q}dV + \oint_S \vec{n}FdS + \Phi = 0 \qquad (5)$$

where $\vec{Q} = (\rho, \vec{m}, \rho e, \rho c_i), i = 1,...n$ vector of conservative unknowns , $c_i = \rho_i / \rho$ - mass concentration of mix component, $\Phi = (0,0,0,0,0, \rho f_i)$ source term , $F = (\vec{m}, \vec{m}\cdot\vec{m}/\rho + PI, \vec{m}(e+p)/\rho, \vec{0})$

Vector of flows , $P = \rho R_B T \sum_i \frac{c_i}{\mu_i}$, $e = R_B T \sum_i \frac{c_i}{\mu_i}/(\gamma - 1) + \vec{V}^2/2 + \sum_i c_i h_i$ - pressure and full energy of volume unit $\sum_i c_i h_i$ - internal energy of chemical reactions.

Numerical simulation where provided for test problems of deflagration initiation from thermal spot and propagation of deflagration front in isolated cylinder and axisymmetrical channels with obstacles for gas mixes methane -air and hydrogen-air. Numerical algorithm [6] was developed on the basis of difference schemes of Harten [7] of second order of accuracy for time and space and Chakravarthy - Osher [8] one of second order of accuracy for time and third order accuracy for space. Aim of calculation providing was simulation of initial stage of deflagration appearing in flows of reacting gas mixes

Numerical simulation of methane -air gas mix deflagration

For specification of flow structure of investigated problem (appearing of deflagration from initial thermal spot in closed cylinder) calculations of methane -air gas mix deflagration where provided on the basis of one-reaction mode (initial molar concentration of methane was 0.4 and thermal spot was situated in outer part of cylinder exclude areas near boundaries):

$$CH_4 + 2O_2 = CO_2 + 2H_2O. \qquad (11)$$

For Arrhenius low $k = A \cdot \exp(-E/RT)$ the next meanings of coefficient from [9] where used: $A = 1.35 \cdot 10^{20}, E = 3. \cdot 10^4 kJ/mol \cdot c$.

On Figure 1, A-C level lines of methane molar concentration are drown (in write column corresponding to **level lines** meanings of concentration **are drown in percentage) and velocity vectors in** consecutive time moments:

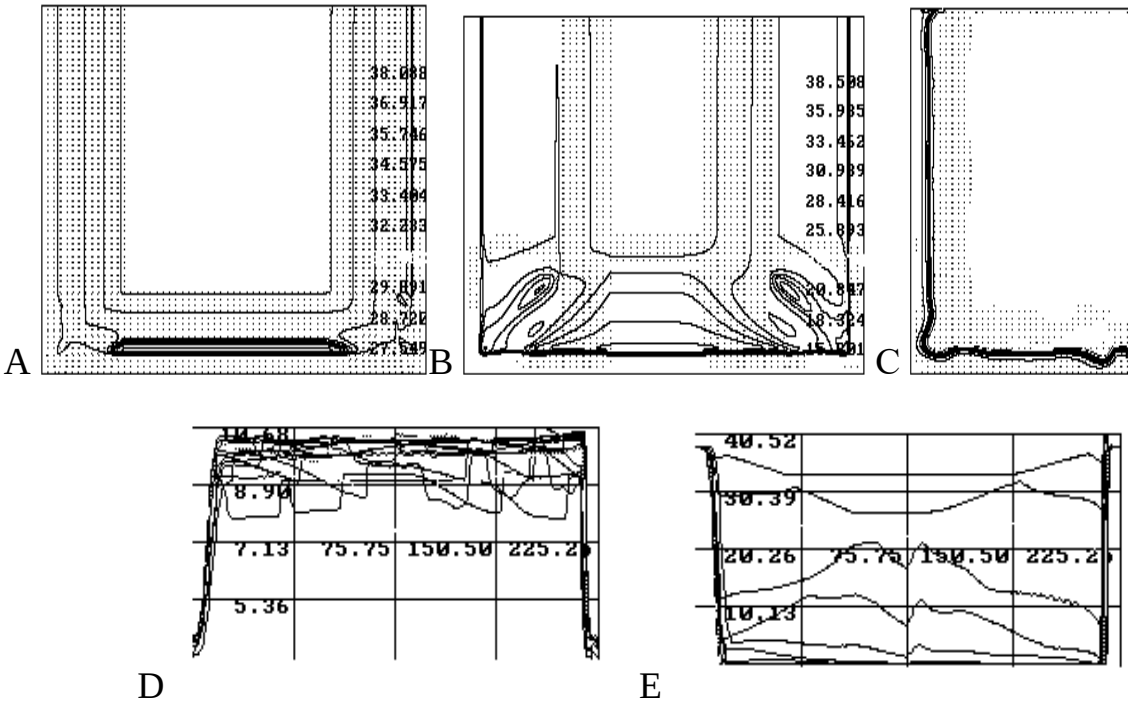


Fig. 1 A-C – level lines of methane molar concentration are drown (in write column corresponding to level lines meanings of concentration are drown in percentage) and velocity vectors in consecutive time moments ; D, E – graphics of temperature and molar concentration in the middle cylinder section in consecutive time moments.

Graphics on figure 1 demonstrate fast deflagration methane and corresponding grows of temperature in closed cylinder.

Numerical simulation of hydrogen -air gas mix deflagration

Two kinetic model where used for numerical simulation of hydrogen - air gas mix deflagration.

1. Model on the basis of full system of kinetic equations with 9 reactions for numerical simulation of slow deflagration

Flow in closed cylinder initiated from thermal spot with T= 550^0 C was calculated on the basis of full system of kinetic equations with 9 reactions (Table 1) with meanings of Arrhenius constants from [10]. Results of calculations on orthogonal grid 300x300 are shown on figure 2.A-C - level lines of temperature and in write column corresponding to level lines meanings of molar concentration in percentage are drown . On figure 2. D, E – graphics of temperature and molar concentration are drown for grid line $i=20$ in consecutive time moments .

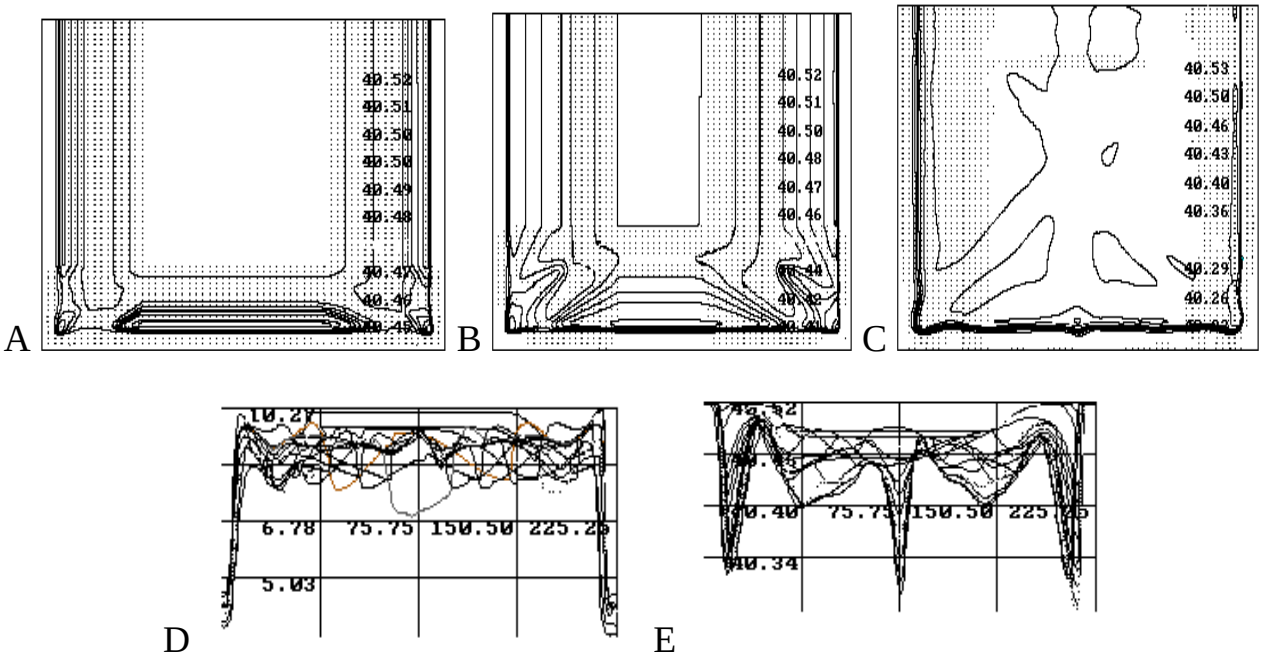


Fig..2 A-C – C - vectors of velocity , level lines of temperature and in write column corresponding to level lines meanings of molar concentration of H_2 in consecutive time moments are drown. On figure 2. D, E – graphics of temperature and molar concentration are drown for grid line *i=20* in consecutive time moments . Calculation where provided on the basis of full system of kinetic equations with 9 reactions.

2. Model on the basis of branching chain reaction [5] for numerical simulation of transition deflagration to detonation .

Flow in closed cylinder initiated from thermal spot with T= 700^0 C was calculated on the basis of model of branching chain reaction with meanings of Arrhenius constants from [5] . On the full time step of numerical algorithm initially simplified differential kinetic equation for concentration of *[H]* was decided numerically separately with small time step (some time step for one time step for solving gas dynamics system (5)). Then with using new meanings of concentration of *[H]* on *n+1* - layer and meanings of concentration $[H_2]$ $[O_2]$ from n-layer we define quasi -stationary concentration of radicals *[O]* and *[OH]* from algebraic equation and finally find solution of system of differential for meanings molar concentration for $[H_2]$, $[O_2]$, $[H_2O]$, $[HO_2]$, $[H_2O_2]$ on the *n+1* time layer . Then we use this meanings of molar concentration of species for solving gas dynamics system of equations (5) on the *n+1* time layer .

Results of calculations on orthogonal grid 300x300 are shown on figure 3.A-C - level lines of temperature and in write column corresponding to level lines meanings of molar concentration in percentage are drown . On figure 3. D, E – graphics of temperature and molar concentration are drown for grid line *i=20* in consecutive time moments .

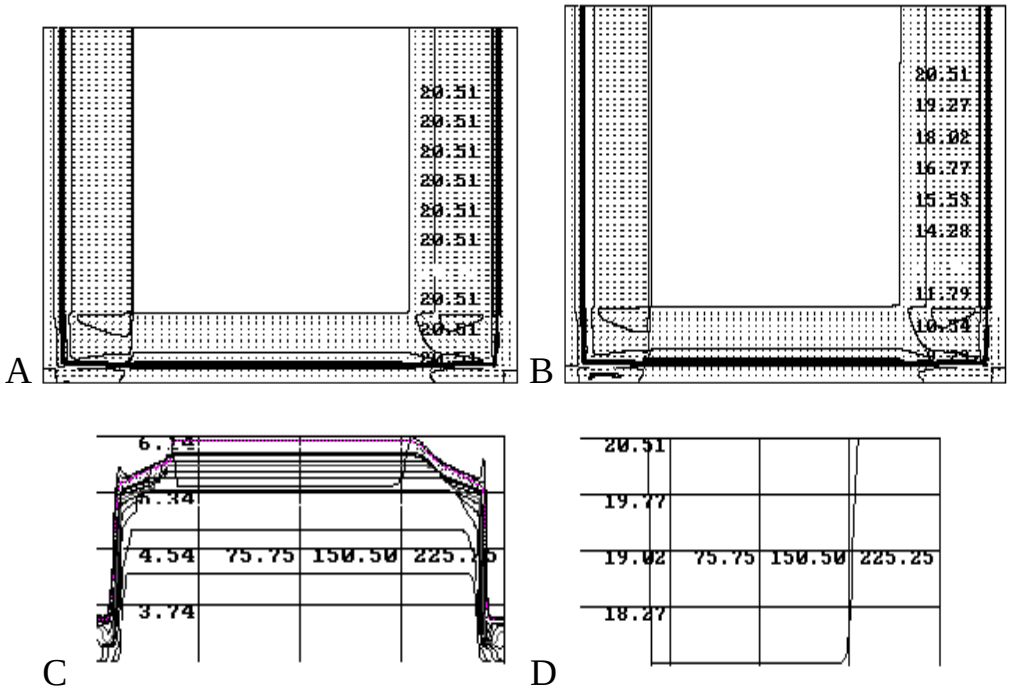
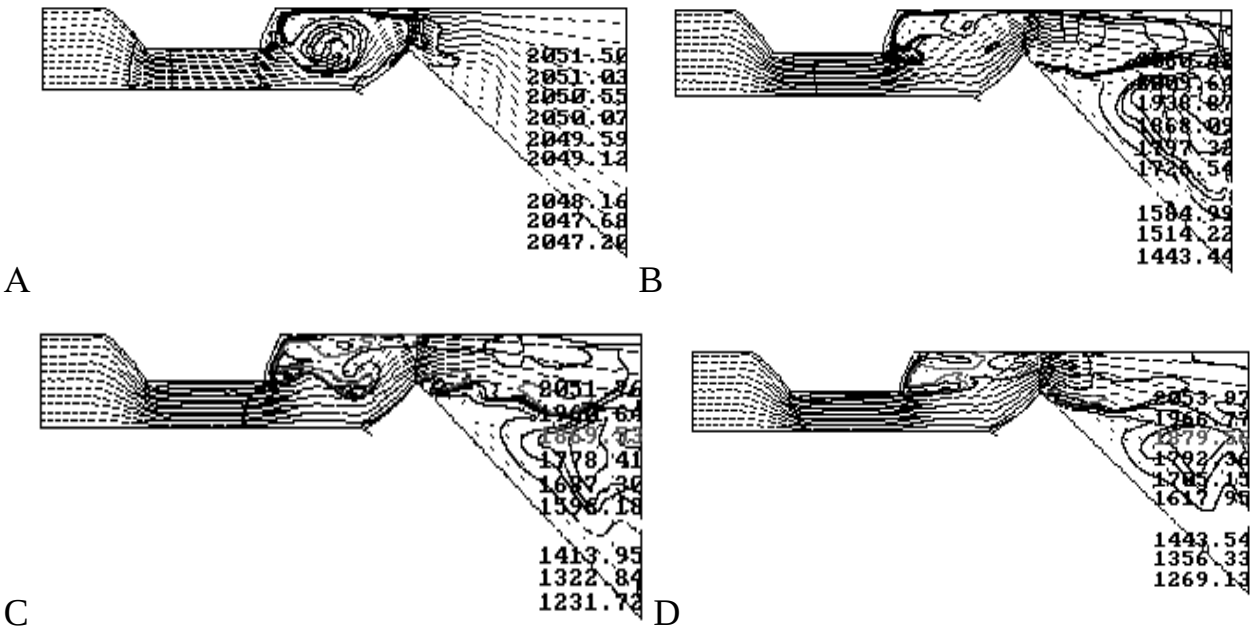
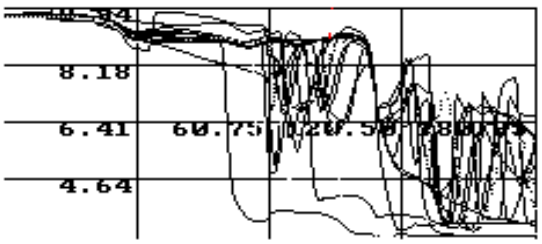


Fig. 3 A-B – A-C -vectors of velocity , level lines of temperature and in write column corresponding to level lines meanings of molar concentration of H_2 in percentage in consecutive time moments are drown . On figure 3. D, E – graphics of temperature and molar concentration are drown for grid line *i=20* in consecutive time moments Calculation where produced on the basis of branching chain reaction [5]

Numerical simulation of flows with transition deflagration to detonation in axisymmetric channels with obstacles where also produced on the basis of branching chain reaction [5] . Form of obstacles are analogous to ones , used in [11], nevertheless geometry of channels essentially different. Thermal spot initiates reaction in left chamber of channel region initially filled by hydrogen-air mixture . Curvilinear structural grids for region of channel where constructed on the basis ob algorithm [12].





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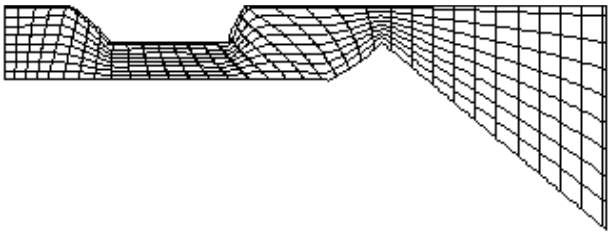

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Рис 4 A-D – vectors of velocity, level lines of temperature and in write column corresponding to level lines meanings of molar concentration of H_2 in percentage multiplied by 100 inside the axisymmetric channel in consecutive time moments are drown.; E – Graphics of temperature for middle grid coordinate line i=50 in consecutive time moments , F – curvilinear structured calculation grid (every 10-th coordinate line is drown). Calculation where provided on the basis of branching chain reaction .

Structure of flow on figure 4, A-D corresponds to deflagration of hydrogen - air mix inside the axisymmetric channel. Condensations of H_2 level lines correspond to fronts of deflagration and transition to detonation ones.

Conclusion

Testing was provided of application kinetic model of branching chain reaction for gas dynamics numerical simulation of initial stage of deflagration and transition to detonation for hydrogen-air mix.

Algorithm was developed of two-velocity calculations with small time step for one ordinary differential equation for [H] concentration and subsequent definition concentrations of the others component of gas mix and and greater time step for numerical decision of gas dynamics system of equation for reactive gas mix on the basis of TVD - schemes of Harten and Chakravarthy - Osher.

On the basis of this algorithm numerical simulations of two test problems where provided: Initiation of deflagration from thermal spot and propagation of deflagration fronts for isolated cylinder and axisymmetric channel with obstacles

Calculations provided demonstrate applicability of developed algorithm for numerical simulations of initial stage of deflagrationof hydrogen-air mixes.

References

1. Levin V A, Markov VV, Osinkin C F *Physica Goreniya y Vzryva* (Moscow) 1995 vol. 31 No 2: 91-95.
2. Levin V.A., Nechaev Y.N., Tarasov A.I., Control of detonation processes. Ed. G. Roy. Moscow, Elex-KM Publishers 197-201, 2000.
3. Zhdan SA. Bykovskii F.A. Vedernikov F.F. Mathematical modeling of a rotating detonation wave in a hydrogen-oxygen mixture. Combustion. Explosion and Shock Waves. 2007, vol. 43 No 4: 449-459.

4. Semenov N N Uspehy Himii . (Moscow), 1967 vol. 36, No1: 3-22.
5. Denisov E T, Sarkisov O M,Lihtenshtein G I 2000 Chemikal Kinetic (Moscow), Himiya. 568 p.
6. Martyushov S.N Computer Technologies (in Russian) 1996, Novosibirsk Vol. 1, No 2: 82-89.
7. Harten A A high resolution scheme for the computation of weak solutions of hyperbolic conservation laws. - J. of Comp. Phys., 1983, Vol. 49, : .357-69.
8. Chakravarthy S.R., Osher S. Computing with High-resolution Upwind Schemes for HyperbolicEquations. Lectures in Applied Mathematics. 1985 Vol. 22 pt.1: 57-86.
9. Kozubkova M., Krutil Y., Nevrliy V., Fizika goreniya i vzrayva (in Russian) ,2014. Vol. 50, № 4: 8-14.
10. Ibragimova L.B., Smechov G.D., Shatalov O.P. Recommended Rate Constants of Chemical reactions in an H2-O2 Gas Mixture with Electronucally Excited Species O2 , O, OH Involved. Institute of Mechanics of Lomonosov Moscow State University, Moscow, 2003.
11. Markov V.V. Initiation and Propagation of detonation waves in channels. Proceedings of 22-nd ICDERS Minsk.. Belarus. 009
12. Martyushov S.N. Construction of Calculation Grids on the Basis of Poisson Equation Decision. 15th IMACS World Congress on Scientific Computation, Modelling and Appl. Maths. Proc. Berlin-1997, V.2, :191-195.