Mini Review

BIOMEDICAL Journal of Scientific & Technical Research

ISSN: 2574 -1241

DOI: 10.26717/BJSTR.2025.61.009585

Comparing of Using Different Systems of Kinetic Equations for Numerical Simulation of Deflagration Initiation in Hydrogen-Air Mixtures Flows

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ARTICLE INFO

Received: March 28, 2025

Published: April 10, 2025

Citation: Martyushov S N. Comparing of Using Different Systems of Kinetic Equations for Numerical Simulation of Deflagration Initiation in Hydrogen-Air Mixtures Flows. Biomed J Sci & Tech Res 61(2)-2025. BJSTR. MS.ID.009585.

ABSTRACT

Abbreviations: ODE: Ordinary Differential Equations

Introduction

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 problem of hydrogen detonation engine constructing 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 of vie process of transition to detonation can be treated as transition from slowly deflagration to branching chain reaction in hydrogen-air mix. Different authors [4-7] used different systems of reactions for numerical simulation of hydrogen-air mixes deflagration. In this paper attempt was made to compare results of using some of these different systems. Coefficients for all reactions, used in this paper where taken from [8].

Kinetic Model

Process of deflagration appearance in hydrogen-air mixes can be treated as transition from slow chemical reactions to fast branching chain reactions. Theory of branching chain reactions was developed by Semenov [4]. Equations of chemical reactions can be presented as follows

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

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

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

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

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

The algorithms for numerical solving of system [2-4] consist of solving fool system of stiff ODE (ordinary differential equations) on the basis of numerical Gear method. Different authors [4-7] used different systems of reactions for numerical simulation of hydrogen-air mixes deflagration. In this paper we try to compare results of using some of these systems. The first system of reaction for hydrogen-air gas mix of 9 component: H_2, O_2, H, O, H_2O, OH, HO_2, H_2O_2, N_2 is the most widespread. The next 9 reactions where choose: Results of numerical decision (for small closed finite volume without gas dynamics effects) of stiff ODE system [2-4] on the basis of Gear method with system of reaction from Table 1 are shown on the Figure 1. Initial meanings of components H_2 =0.2 of molar amounts of mix, O_2 =0.1 of molar amounts of mix, N_2 =0.7 of molar amounts of mix, initial concentration of H_2 O =0., final meanings of H_2 O 0,2 of molar amounts of mix. During the calculation time changes from 0 to 12 sec. Calculation began with temperature T=3.3Tatm, and it changes during calculation in connection with heat effect of chemical reactions. From this example and the next ones can be seen that appearance of significant amount of radical H_2 O_2 in gas mix lead to fast speed of changing for main components (H_2, O_2 and H_2 O), that demonstrate deflagration initiation. The second system of reactions (situated in Table 2) was system of 13 reactions for the same components H_2, O_2, H, O, H_2O, OH, H O_2, H_2O_2, N_2: Results of numerical decision of stiff ODE system [2-4] on the basis of Gear method with system of reaction from Table 2 are shown on the Figure 2. Initial meanings of components H_2 =0.2 of molar amounts of mix, O_2 =0.1 of molar amounts of mix, N_2 =0.7 of molar amounts of mix, initial concentration of H_2 O =0., final meanings of H_2 O 0,2 of molar amounts of mix. During the calculation time change from 0 to 9 sec. Calculation began with initial temperature T=3.25Tatm. The third system of reactions (situated in Table 3) was system of 28 reactions-with one additional component O_3: Results of numerical decision of stiff system of ODE [2-4] on the basis of Gear method with system of reaction from Table 3 are shown on the Figure 3. Initial meanings of components H_2 =0.2 of molar amounts of mix, O_2 =0.1 of molar amounts of mix, N_2 =0.7 of molar amounts of mix, initial concentration of H_2 O =0., final meanings of H_2 O 0,2 of molar amounts of mix. During the calculation time change from 0 to 9 sec. Calculation began with temperature T=3.1Tatm, and it changes during calculation in connection with heat effect of chemical reactions.

Table 1: The first system of chemical reactions.

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

Table 2: The second system of chemical reactions.

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

Table 3: The third system of chemical reactions.

$H_2 + O_2 = 2OH$	$H_2 + OH = H + H_2O$	$2HO_2 = H_2O_2 + O_2$
$H + O_2 = O + OH$	$H_2 + O = H + OH$	$O_2 + M = 2O + M$
$H_2 + M = 2H + M$	$H_2O_2 + M = 2OH + M$	$OH + H_2O = H + H_2O_2$
$O_3 + M = O_2 + O + M$	$OH + M = O + H + M$	$H_2O + M = OH + H + M$
$HO_2 + M = O_2 + H + M$	$H_2 + O_2 = H + HO_2$	$H_2 + 2O_2 = 2HO_2$
$H_2 + HO_2 = OH + H_2O$	$H_2 + H_2O_2 = H_2O + H + OH$	$H_2 + HO_2 = H + H_2O_2$
$O_2 + H_2O = O + HO_2$	$2O_2 = O_3 + O$	$OH + O_2 = HO_2 + O$
$OH + O_2 = O_3 + H$	$2OH = O + H_2O$	$2OH = H + HO_2$
$HO_2 + O_3 = OH + 2O_2$	$OH + HO_2 = O_2 + C$	$OH + H_2O_2 = HO_2 + H_2O$
$O + H_2O_2 = OH + HO_2$		

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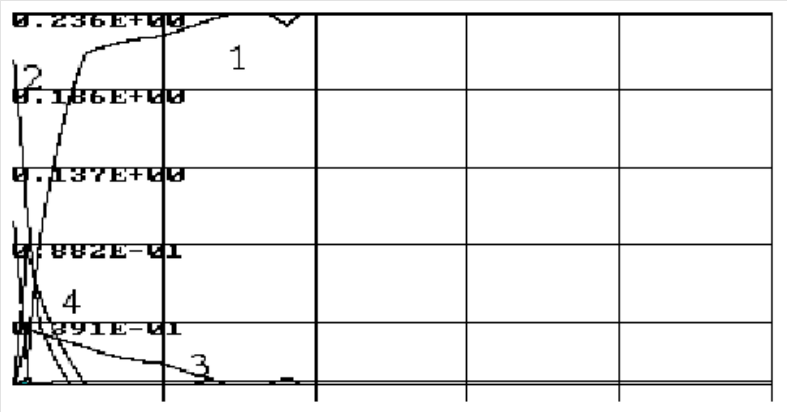

Figure 1: Graphics of changing concentrations of mix components with time (time scale from 0 to 12 sec.), graphic 1- concentration of H_2O, 2 - concentration of H_2, graphic 3 - concentration of H_2O_2, system of reactions is taken from Table 1.

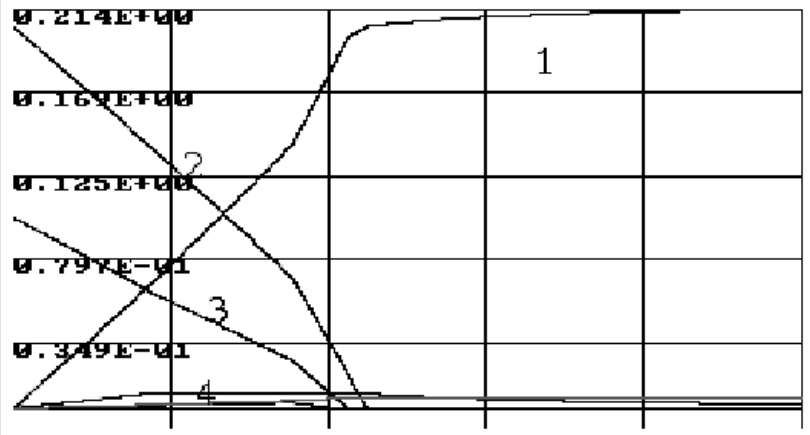

Figure 2: Graphics of changing concentrations of mix components with time (time changes from 0 to 9 sec.), graphic 1- concentration of H_2O, 2 - concentration of H_2, graphic 3 - concentration of O_2, graphic 4 - concentration of H_2O_2, system of reactions is taken from Table 2.

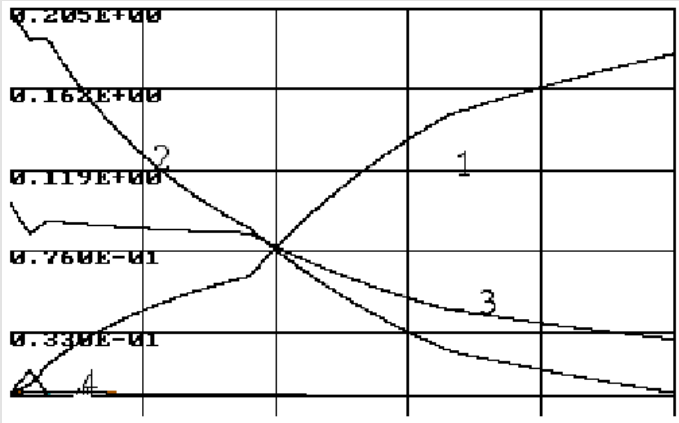

Figure 3: Graphics of changing concentrations of mix components with time (time scale from 0 to 9 sec.), graphic 1- concentration of H_2O, 2 - concentration of H_2, graphic 3 - concentration of O_2, graphic 4 - concentration of H_2O_2., system of reactions is taken from Table 3.

Numerical Simulation of Reactive Gas Mixes Flows

In this paragraph we compare using of systems of reactions from Table 2 and Table 3 for numerical simulation of deflagration appearance in hydrogen – air gas mixtures flows. Numerical simulations of deflagration appearance in hydrogen – air gas mixtures flows with using system of reactions from Table 1 can be found in, for example, in [4-7] and previous papers of author [9]. 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:

$$d / dt \int_v \vec{Q}\, dv + \oint_s \vec{n} F dS + \phi = 0 \qquad (5)$$

where $\vec{Q} = \left(\rho, \vec{m}, \rho e, \rho c_i\right), i = 1,...n$ 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,

$F = \left(\vec{m}, \vec{m}.\vec{m}/\rho + PI, \vec{m}(e+p)/p, \vec{0}\right)$ vector of flows,

$p = \rho R_B T \sum_i \frac{c_i}{\mu_i}$ $\dot{e} = R_B T \sum_i \frac{c_i}{\mu_i} / (\gamma - 1) + V^{2r} / 2 + \sum_i c_i h_i$, - pressure and full

energy of volume unit,

$\sum_i c_i h$ -internal energy of chemical reactions.

Examples of Numerical Simulation of Flows with Deflagration Appearance

Numerical simulation where provided for test problem of deflagration initiation from spreading shock wave of intensity of Msh and initiating of deflagration front in isolated cylinder for hydrogen-air gas mixes. Numerical algorithm [9] was developed on the basis of pure upwind variant of difference scheme Chakravarthy - Osher [10] second order of accuracy for time and third order accuracy for space. Aim of providing calculation was simulation of initial stage of deflagration. The first example consist of numerical simulation deflagrarion initiation in hydrogen – air gas mixtures flow behind shock wave intensity Msh=3.5 (calculations was provided with stable shock wave and appropriate velocity of flow before shock) for system of chemical reactions from Table 2 (Figure 4). The second example just the same consist of numerical simulation deflagrarion initiation in hydrogen – air gas mixtures flow behind shock wave intensity Msh=3.5 (calculations was provided with stable shock wave and appropriate velocity of flow before shock) for system of chemical reactions from Table 3 (Figure 5).

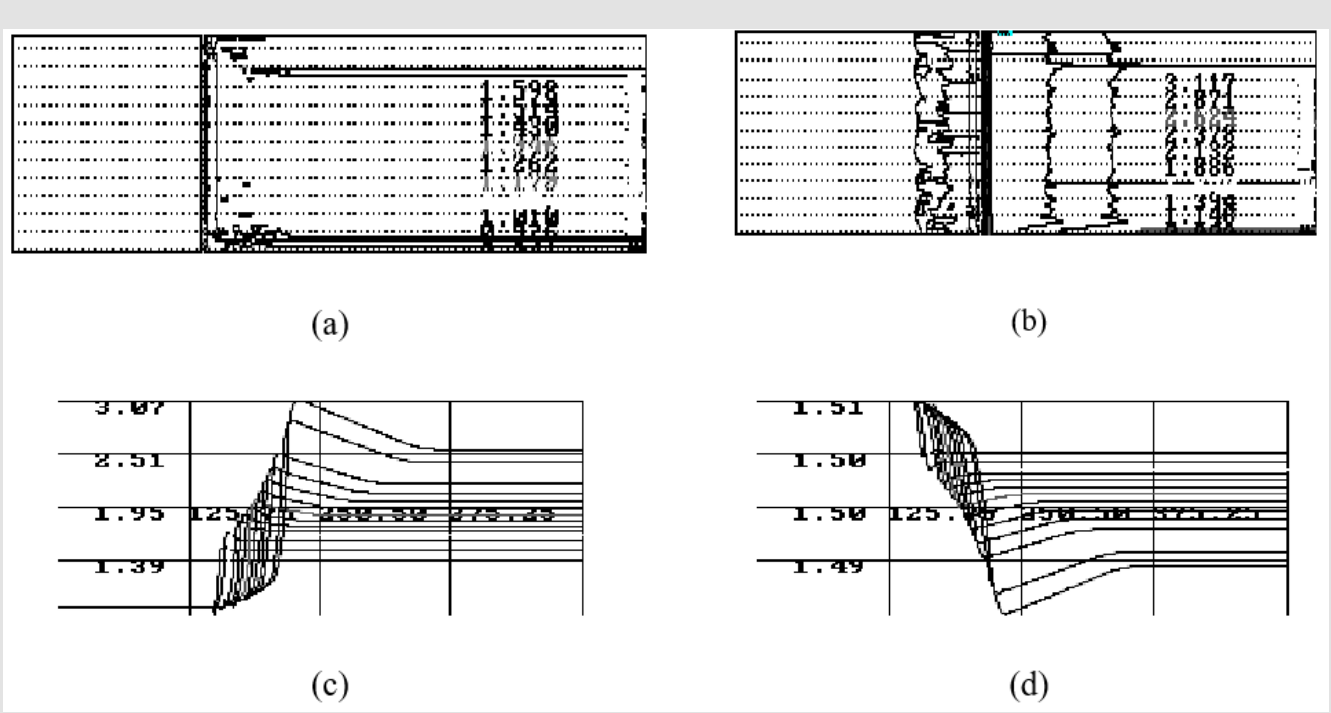

Figure 4: (a), (b) – vectors of velocity, level lines of water concentration and in write column corresponding to level lines meanings of water concentration (in percent of whole molar number) in time moments t_0 =0 sec and t_{fin}=7.5 sec; (c), (d) – graphics water concentration (c) and concentration of O_2 (d) along bottom boundary of the cylinder in consequent time moments (14 time points from 0. till 8.5).

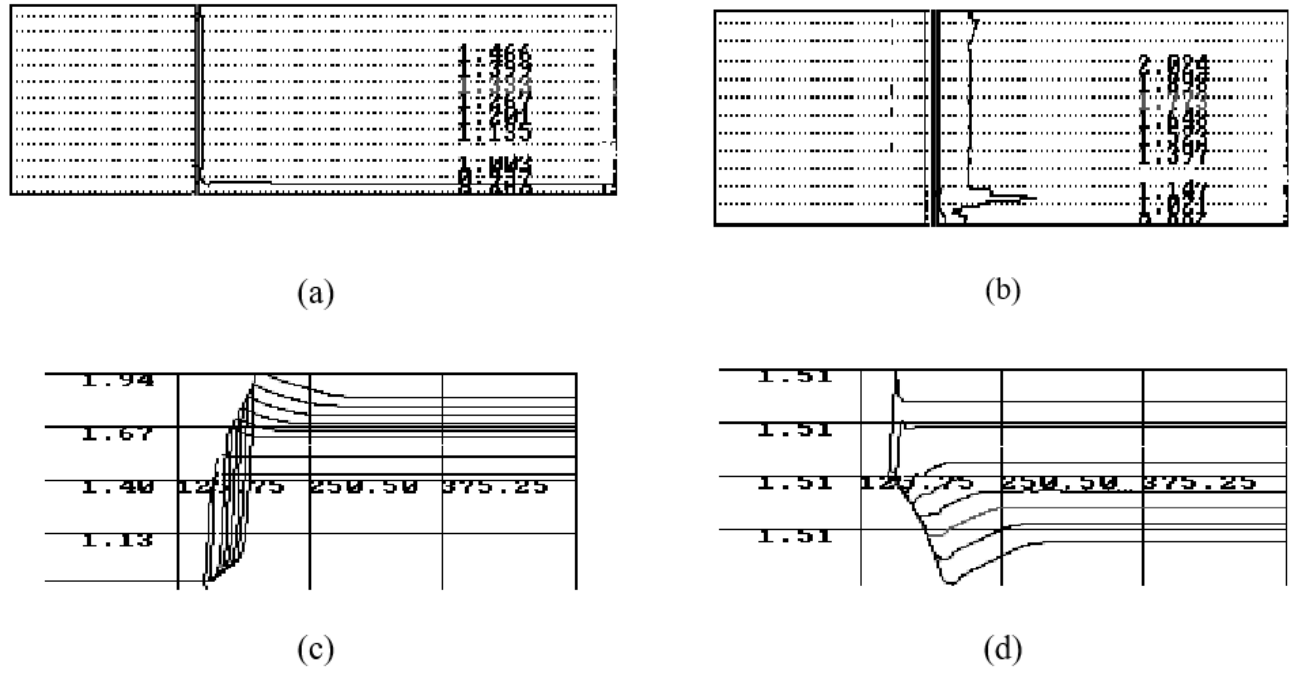

Figure 5: (a), (b) – vectors of velocity, level lines of water concentration and in write column corresponding to level lines meanings of water concentration (in percent of whole molar number) in time moments t_0=0 sec and t_{fin}=8.5 sec; (c), (d) – graphics water concentration (c) and concentration of O_2 (d) along bottom boundary of the cylinder in consequent time moments (14 time points from 0. till 8.5).

Summary

Three test variants of numerical solution of system of stiff ODE [2-4] for system of reactions from Table 1, Table 2 (9 components, 9 and 13 reactions) and Table 3 (10 components, including O3 and 28 reactions) where provided. Proposal was used that process of deflagration initiation realized in one small closed finite volume without gas dynamic effects. For testing possibility of using system reactions from Table 2 and system reactions from Table 3 in gas dynamic numerical simulation of flows with hydrogen-air deflagration two variants for one gas dynamic problem was calculated. Gas dynamic problem consist of deflagration initiation behind stable shock wave of intensity Msh 3.5 in cylinder. (Possibility of using system reactions from Table 1 was shown previously in numerous calculations of different authors, see [4-7] and author himself [9]).

Results of provided calculations demonstrate possibility of using system reactions from Table 2 and system reactions from Table 3 in gas dynamic numerical simulation of hydrogen-air deflagration. This results didn't show preferences of using system reactions from Table 2 and Table 3 before using system reactions from Table 1. Nevertheless, using systems reactions from Table 2 and Table 3 provide additional possibilities for solving other problems in numerical simulations of gas dynamics flows with deflagration..

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ISSN: 2574-1241

DOI: 10.26717/BJSTR.2025.61.009585

Martyushov S N. Biomed J Sci & Tech Res

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