Mathematical modeling of detonation initiation and propagation in the complex-shaped domains

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Abstract. The present work is devoted to the development of the numerical algorithm for the mathematical modeling of gaseous detonation initiation and propagation and the complex-shaped domains using fully unstructured computational grids and high-order numerical schemes. Mathematical model is based on two-dimensional Euler equations supplemented with the one-stage chemical kinetics model. Numerical algorithm is based on the finite volume approach, AUSM numerical flux and the reconstruction of the grid-functions on unstructured grids. The canonical problem of cellular detonation formation is considered as the test case. The influence of grid resolution and the properties of the numerical scheme on the results of modeling is investigated. The problem of the critical geometrical conditions determination for the detonation initiation and propagation in the asymmetrical tube with variable cross-section area filled with stoichiometric hydrogen–air mixture is considered. The problem in consideration relates to the utilization of the industrial waste.

1. Introduction
Mathematical modeling of two-dimensional flows with detonation waves (DWs) as a result of the solving of the Euler equations for an inviscid gas supplemented by a chemical reaction kinetics model originates in the late seventies [1, 2]. Since then, with the development of computational methods for solving gas dynamics problems, the improvement of kinetic schemes and the growth of available computing powers, continuous refinement of qualitative and quantitative process characteristics have been occurred (for example, obtaining the three-dimensional spin mode of propagation, the thin structure of the cellular detonation, the detonation limits). One can agree with the paper [3], in which the current understanding of the mechanisms of the DW propagation is put into direct dependence on the maximum computer performance achieved at the moment. At the same time, the growth of computational power and, as a result, the possibility to carry out calculations with more and more detailed spatial-temporal resolution revealed a number of unusual effects of the detonation modeling, that yet have not had a full explanation. The effects include the possible detonation damping for kinetics parameters close to hydrocarbon fuels in two-dimensional calculations of the DW long distribution in the plane channel [4]. Thus, despite, the almost forty-year history of computational works in the detonation field, a number of fundamental questions of DW mathematical modeling remain.

A particular problem is to study the problems of initiation and propagation of DWs in areas with complex shapes and curvilinear boundaries. Such problems arise in a large number in the study of explosion safety problems, the development of promising power facilities and energy
systems [4–6]. In the context of this study, the computational technologies used by the authors in similar calculations are of interest. So, in papers [4, 5] for carrying out three-dimensional computations of initiation and propagation of DW in domains with complex forms the block-structured grids, the classical first approximation order (AO) scheme of S K Godunov [5] or its modification with use of some interpolation schemes for increase of approximation order [4] are applied. At the same time, with respect to the gas dynamics problems of chemical inert media including shock wave problems, the apparatus of high approximation order schemes on completely unstructured computational grids have been developed by now (for example, see the well-known work [7]). The analysis of publications on the application of such approaches to the study of high-speed flows with chemical reactions yields a very small number of papers [8–10], with the finite element approach applied in [9, 10]. The most probable reason is the fact that although the integration of the gas dynamics equations is a key element of the computational algorithm for calculating high-speed flows with chemical reactions, the presence of strongly nonlinear sources in the right-hand sides of the equations significantly narrows the possibilities of using many numerical methods that successfully come with the problems of the gas dynamics of inert media.

The aim of the work is the development of the computational algorithm of the second AO on a completely unstructured grid for calculations of two-dimensional flows with DWs applicable for the modeling flows in areas of various forms and testing the algorithm on solving the canonical problem of forming the cellular structure of DW. The developed algorithm will be applied to the modeling of the facility for utilization of used automobile tires [11, 12].

2. Problem statement and mathematical model for the planar detonation wave propagation simulation

The problem of initiation and propagation of DW in a plane channel of width \( H \) and length \( L \) with rigid impermeable walls is considered. The detonation is initiated as a result of instantaneous energy release in the domain of the length \( l \), adjacent to the left channel wall. At the initial time, the channel is filled with a resting reactive gas with pressure \( p_i \) and density \( \rho_i \). The values of initiation parameters near the left channel wall are \( p_i \) and \( \rho_i \).

The mathematical model is based on the two-dimensional system of Euler equations written in the Cartesian frame \((x, y)\) in vector divergent form supplemented by the global model of the chemical reaction kinetics:

\[
U_t + F_x + G_y = S,
\]

\[
U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho Z \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ (e + p) u \\ \rho Z u \end{bmatrix}, \quad G = \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ (e + p) v \\ \rho Z v \end{bmatrix}, \quad S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \rho \omega \end{bmatrix}, \quad (1)
\]

\[ e = \frac{\rho w^2}{2} + \rho \varepsilon, \quad \varepsilon = \frac{p}{\rho(\gamma - 1)} + ZQ, \quad \omega = -AZ \exp \left( -\frac{Eho}{p} \right). \]

Here and further, the notations are standard, \( Q \) is the heat release of the chemical reaction, \( Z \) is the mass fraction of the reactant in the mixture, \( \omega \) is the chemical reactions rate, \( A \) is the pre-exponential factor, \( E \) is the activation energy of the mixture. Also, the perfect gas model with specific heat ratio \( \gamma \) is used.

The system of governing equations is converted to the nondimensional form in accordance with [13]. We use the density and pressure of the gas in front of the DW as the characteristic scales: \( \rho_{\text{ref}} = \rho_i, \rho_{\text{ref}} = p_i \). The velocity scale is \( w_{\text{ref}} = \sqrt{\rho_i/\rho_a} \). The heat release of the chemical reaction is scaled by \( w_{\text{ref}}^2 \), the activation energy is scaled by \( \mu w_{\text{ref}}^2 \), where \( \mu \) is the molar mass of the gas. The length scale is chosen to be equal to the half-reaction zone length \( l_{1/2} \) of
the ideal planar detonation [14]. In the selected units, physical and chemical properties of the reacting mixture are completely determined by specifying three dimensionless parameters ($\gamma$, $Q$ and $E$). This fact makes the applied ideology attractive for the theoretical studies of different regimes of DW propagation. For example, for the parameters $\gamma = 1.2$, $Q = 50$, $E = 25$ we obtain a stable DW (in the sense that the solution of the ideal planar detonation proves to be stable in the linear approach), for $E = 26$ we obtain a weak-unstable one, for $E = 28$ we obtain irregular one, for $E = 35$—strongly unstable one [13,15–17]. Further, in this paper, we consider the case of $E = 25$.

3. Computational algorithm
The main feature of the computational technique is the use of completely unstructured grids with triangular cells. A Delaunay triangulation based on the arrangements of the computational grid nodes to satisfy the Delaunay condition is carried out to construct the grid. The grid resolution is determined by the number of nodes per half-reaction zone length $l_{1/2}$. All triangles of the computational grid are numbered in a pass-through manner.

The computational algorithm is based on the principle of splitting into physical processes [18]. When passing from one time layer to another one, one first integrates the equations of gas dynamics without considering the execution of chemical reactions [$S = 0$ in (1)], and thereby performing the first stage of the splitting procedure. The second stage involves the contribution estimation of the chemical reactions without considering the convection (the second stage of splitting).

The spatial part of system of equations (1) is discretized using the finite volume method at the gas dynamics stage of the algorithm:

$$\frac{\partial U}{\partial t} \equiv L(U) = -\frac{1}{S_k} \sum_{\sigma=1}^{3} (F_{k,\sigma} l_{k,\sigma}) .$$

Here, the spatial index $k$ corresponds to the number of calculated cell of area $S_k$, the summation is conducted on all edges $\sigma$ of the cell $k$, $l_{k,\sigma}$ is the length of the edge with the index $\sigma$, $F_{k,\sigma}$ is the vector of numerical flux through the edge in the direction of the unit normal $n_{k,\sigma} = (n_{k,\sigma x}, n_{k,\sigma y})$ that is external to the edge. To calculate the flux

$$F_{k,\sigma} = F_{k,\sigma} (U^n_{k,\sigma}, U^r_{k,\sigma})$$

we pass from the initial global frame $(x, y)$ to the local one, that is associated with the outer normal $n_{k,\sigma}$ to the edge $\sigma$ and the tangent vector $\tau_{k,\sigma} = (-n_{k,\sigma y}, n_{k,\sigma x})$. The flux in the local frame is calculated using the AUSM scheme [19] extended for the case of a two-component mixture.
Figure 2. Initiation and propagation of the DW in the plane channel from (a) calculation No. 1; (b) calculation No. 2; (c) calculation No. 3; (d) calculation No. 4. “Numerical soot footprints”.

To increase the AO, the following reconstruction of the grid functions is applied [20]. In the local coordinate system, the numerical flux is calculated by the parameters on left and right side with respect to the discontinuity (figure 1):

\[ U_{n_{\sigma}}^L = T_{n_{k,\sigma}} U_{n_{k,\sigma}} = \frac{1}{2} \Psi \left( T_{n_{k,\sigma}} U_{k} + T_{n_{k,\sigma}} U_{k,A} - T_{n_{k,\sigma}} U_{k,B} - T_{n_{k,\sigma}} U_{k,\sigma} \right), \]

\[ U_{n_{\sigma}}^R = T_{n_{k,\sigma}} U_{n_{k,\sigma}} = -\frac{1}{2} \Psi \left( T_{n_{k,\sigma}} U_{k} - T_{n_{k,\sigma}} U_{k,A} + T_{n_{k,\sigma}} U_{k,B} + T_{n_{k,\sigma}} U_{k,\sigma} \right), \]

\[ U_{n_{k,A}} = \frac{1}{|C_A|} \sum_{i \in C_A} U_{n_i}, \quad U_{n_{k,B}} = \frac{1}{|C_B|} \sum_{i \in C_B} U_{n_i}. \]

Here A denotes the set of triangles that have a common node (vertex) with the triangle \( k \) where the node is an opposite to the edge \( \sigma \). Similar B denotes the set of triangles that have a common node (vertex) with the triangle \( k, \sigma \) where the node is an opposite to the edge \( \sigma \). The minmod limiter [21] and van Leer [22] limiter are considered as a limiter function \( \Psi \):

\[ \Psi_{\text{minmod}}(a, b) = \frac{1}{2} \text{sign}(a + b) \min(|a|, |b|), \quad \Psi_{\text{vanLeer}}(a, b) = (\text{sign}(a) + \text{sign}(b)) \frac{|ab|}{|a| + |b| + \phi}. \]
In the case when the arguments of the function of the limiter are vectors, the limiter is applied component-wise. In the calculations with van Leer limiter the small value parameter in the denominator was taken equal to $\phi = 10^{-5}$.

Time integration is carried out using explicit Runge–Kutta method of the second AO:

$$U_k^{(1)} = U_k^n + \tau^n L_k(U^n),$$

$$\tilde{U}_k^{n+1} = \frac{1}{2} U_k^n + \frac{1}{2} U_k^{(1)} + \frac{1}{2} \tau^n L_k(U^{(1)}).$$

The upper tilde denotes that the obtained solution is the results of the first stage of the splitting procedure. The time integration step $\tau^n$ is chosen from the stability condition [23].

The second stage of the algorithm involves solving a system of ordinary differential equations describing the chemical reactions passing in each cell $k$ of the computational grid.

4. Cellular detonation modeling

Let us consider the initiation and propagation of DW in a plane channel of width $H = 20$ and length $L = 250$, filled with a resting reactive mixture characterized by the following parameters $\gamma = 1.2, Q = 50, E = 25$. All the parameters are dimensionless, see section 2, and correspond to the stable regime of DW propagation. Detonation is initiated as a result of instantaneous energy release in a short region of the length $l = 6.0$ and the entire width of the channel that adjacent to the channel left wall. In this region, the higher values of density $\rho_1 = 3.0$ and pressure $p_1 = 60.0$ are set at the initial time moment with respect to rest of the channel. The computations are performed using the computational algorithms of both first and second AO schemes for both types of limiters on two grids, one of which is called “rough” (about 1.7 million triangular cells), and another is called “detailed” (about 3.5 million triangular cells). In the case of a rough grid, the spatial resolution is about 10 points per length scale $l_1/2$, in the case of the detailed mesh the resolution is about 14 points per length scale. The study of the influence of the Kelvin–Helmholtz and Richtmyer–Meshkov hydrodynamics instabilities on the cellular detonation formation demands at least 300 points per $l_1/2$, as shown in [24] for a similar model mixture, but with a much lower activation energy. To describe the process of interaction of vortex structures with discontinuities which leads to the formation of secondary structures and irregular detonation cells, the study already demands 600 points per $l_1/2$. This paper has no a goal to reach such record resolutions; the focus is on the features associated with the application of unstructured computational grids. The numbering of the part of the numerical experiments, which will be analyzed further, is presented in table 1. The Courant–Friedrichs–Lewy number CFL is taken to be 0.8 in time step calculations in all computations unless otherwise specified.

The energy in the initiation region is enough for the formation of an overdriven planar DW, which begins to propagate in the channel. To visualize the flow pattern we use “numerical soot
Table 1. Parameters of computational experiments.

| No. | approximation order | grid resolution     | limiter  |
|-----|----------------------|---------------------|----------|
| 1   | 1                    | 10 points per $l_{1/2}$ | —        |
| 2   | 2                    | 10 points per $l_{1/2}$ | minmod   |
| 3   | 1                    | 14 points per $l_{1/2}$ | —        |
| 4   | 2                    | 14 points per $l_{1/2}$ | minmod   |

Figure 4. The average velocity of the DW along the symmetry axis of the tube, $l = 30$ cm. The dashed line indicates the CJ velocity of the DW.

footprints”, figure 2. To construct it, the maximum pressure in each cell for the entire time bears in mind. Such visualization corresponds to the experimental method of DW multidimensional structures recording using the smoked foil or plates installed on the wall of the channel that is applied for DW propagation. Approximately at the same distance from the initiation region—about 80 units—in all computations, the front of DW stops being plane, and the system of transverse waves, typical for two-dimensional detonation, appears. In the computations for the appearance of this structure, we do not use any disturbing factors. The trigger to the emergence of so-called DW cell structure is the unstructured type of computational grid that leads to the appearance of small vertical components of gas velocity. At the same time it is known that even in case of uniform computational grid with rectangular cells the cellular structure is formed in the same manner and the triggering mechanism in this case is a set of errors of machine calculations [4, 25]. Despite the fact that the appearance of detonation cells is due to the arbitrary factors, the characteristic scale of the transverse size cells is already determined by the macroscopic parameters of the problem that is typical for the problems of the development of the hydrodynamic instability. In all computations, the transverse cell size tends to increase as DW propagates. In the computation No. 1, after the DW front stops to be plane a regime with three regular detonation cells is generated. In process of DW propagation in the channel, the transient regime with two-three cells is formed. The mesh resolution and low AO do not allow us to obtain characteristic structures in the form of a pair of weak transverse tracks diverging from
the triple point of the transverse waves collision, as one can see in figure 2(d). The mechanism of the appearance of these weak traces is discussed in [25]. It is noted that the extremely high pressure generated by the collision of triple points give rise to the compression waves moving downstream along the transverse shock and forming the weak transverse tracks. The results of the computations No. 2 and No. 3 do not have qualitative differences with the results of the computation No. 1. Using the detailed mesh and the computational algorithm of the second AO (computation No. 4) one can observe that the transitional regime ends with the formation of two transverse waves and one pronounced detonation cell over the entire channel width.

5. Modeling of the facility for utilization of used automobile tires

Let us consider the axisymmetric tube of a variable cross-section, which is filled by quiescent stoichiometric hydrogen–air mixture under the normal conditions, figure 3, that simulates the facility for utilization of used automobile tires [11,12]. The geometry of the problem corresponds to that considered in [12]. The tube consists of a short narrow segment for detonation initiation (preliminary chamber), a conical part for DW passing into a segment of a larger diameter (detonation chamber) and a working chamber. The cases of different expansion angles of the conical part corresponding to the values \( l = 10, 30 \) and 50 cm are investigated. For detonation initiation, the pressure of 40 atm and temperature of 1500 K are set in a region with length 4 cm (colored gray in figure 3). The boundary conditions of impermeability are set on all boundaries of the calculation region. The pressure is recorded by the sensors D1 and D2. The objectives are the description of the mechanism of the development of detonation process in such geometry, the comparative analysis of the pressure curves on sensors under variation of the geometrical parameter \( l \), comparing the results with data from [12] and the research of applicability of the developed computational algorithm of second approximation order on completely unstructured computational grids for solving practical tasks.

The mathematical model is based on the two-dimensional system of Euler equations written in the cylindrical coordinate system \((r, z)\) with taking into account the assumption of the axial symmetry of the flow, supplemented by one-stage kinetics of hydrogen combustion in the air [26]. The computations are carried out on computational grids with cells number between 3 and 4 million depending on the geometry. Because of the large scale of the considered problem, the grid resolution is too coarse with respect to the half-reaction length in the stationary Zeldovich–von Neumann–Doering solution for the considered kinetics model (0.2 mm) in order to obtain effects associated with the DW front instability, but sufficient for estimating the integral gas dynamics parameters of the problem. The numerical method of the second approximation order in time and space is used.

Let us characterize the process evolution for each considered geometry noting the similar and different details. The direct initiation of detonation in the preliminary chamber leads to the overdriven regime of DW propagation, figure 4. The pressure of the rarefaction wave when DW enters the conical part is being reduced from 30 atm to the pressures close to the Chapman–Jouguet (CJ) pressure. Long away behind the DW front, the relatively weak transverse waves are being formed. Much more powerful transverse wave is being formed when DW passing from the conical part of the detonation chamber to a segment of a constant cross-section.

In the case of \( l = 50 \) cm, the DW first reaches the side wall of the working chamber, then the interaction of the DW with the end wall occurs, figure 5(c). In the case \( l = 30 \) cm these events occur at the same time moment, figure 5(b). In the case \( l = 10 \) cm the DW first reaches the end of the channel, figure 5(a). The cumulation pattern of the reflected wave is the most complicated since the wave interacts with the set of transverse waves which were formed in the conic expansion part. Further stages of the process include the convergence of the waves reflected from the end and the side wall of the working chamber and the achievement of a jet formed as a result of the cumulation of the wave, which is formed when the DW passing from
Figure 5. Predicted pressure profiles after DW output into the working chamber at $l = 10$ (a), 30 (b) and 50 cm (c). The coordinate axes are in meters; the pressure values are in atmospheres.

Figure 6. Pressure curves at the sensors (a) D1 and (b) D2. The solid lines are the authors’ computations, the dashed lines are the computations from [12].

the conic part of the detonation chamber to the constant cross-section chamber, the end wall of the working chamber. The cumulation of the wave on the symmetry axis of the tube occurs
at different points of time with respect to the moment of DW arrival to the end of the working chamber for different tube configurations.

Figure 6 illustrates the comparison of the pressure curves on the sensors D1 and D2 with the data from [12]. The curves are matched at the moment of the arrival of the DW at the sensors since there is no exact information about the initiation parameters in [12]. The peak pressure at the sensor D2 is approximately 2 times higher than the analogous value at the sensor D1, because of the interference of the waves reflected from the side and end walls of the working chamber. For each of the three considered configurations, the pressure impulses applied to the end wall of the working chamber were measured by calculating the area under the pressure curve on the sensor D1. The greatest impulse is realized in the case of $l = 50$ cm. In the case of the smallest angle of the conical expansion part, the DW undergoes the least attenuation when the DW passes into the working chamber, in comparison with the other configurations. In the case $l = 30$ cm the impulse is reduced by 6%. In the case $l = 10$ cm the impulse is reduced by 13%.

6. Conclusions

So, the work demonstrates the possibility of numerical modeling of initiation and propagation of gaseous DWs in the two-dimensional statement on completely unstructured computational mesh with triangular cells. The computational algorithm based on the finite volume method of second AO with respect to spatial coordinates is presented and described in detail. On the example of cellular detonation propagation in the model mixture whose chemical reactions are described by one-stage kinetics the work demonstrates that the usage of the minmod limiter provides a stable computation, while the van Leer limiter is unstable. The problem of detonation initiation in the plane channel with the subsequent formation of the cellular structure for two meshes with a resolution of about 10 points per scale and about 14 ones using the computational algorithms of first and second approximation order with respect to spatial coordinates is considered. The computations demonstrate the dynamics of output from the overdriven regime to the Chapman–Jouguet level with the gradual increase in the transverse size of a detonation cell. On the basis of the most detailed mesh using the second order approximation algorithm, the regime with one detonation cell on the entire channel width was obtained.

The work also demonstrates the efficiency of the suggested computational algorithm of second approximation order for calculation two-dimensional axisymmetric flows with detonation waves within the global chemical kinetics model on completely unstructured computational grids to solve the large-scale problem of modeling a facility for crushing tires. The correctness of the obtained results is confirmed by the comparison of the parameters of the self-sustaining detonation wave with analytic estimates of the Chapman–Jouguet parameters and the comparison with the calculated results of other authors. The mechanisms of the process development for three device configurations are described. The pressure impulse acting on the end wall of the working chamber is maximal at the minimum angle of the conical expansion of the detonation chamber.

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