Application of dissipation-free numerical method
CABARET for solving gasdynamics of combustion and detonation

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Abstract. This paper discusses capabilities of the novel dissipation-free CABARET numerical algorithm to solve the range of complex non-stationary combustion problems. On the basis of detailed analysis of the obtained results and comparison with the data derived with the classic low-order coarse particles method it was shown that reactive flow evolution process may be strongly influenced by the artificial effects introduced by the numerical algorithm, numerical dissipation in particular. Revealed peculiarities of the flame propagation dynamics regimes taking place in considered tests allowed us to propose a number of requirements which should be taken into account when choosing numerical procedure suitable for modelling combustion processes in real technical environment.

1. Introduction
Increase in modern computational facilities performance continuously expands the range of problems that could be solved by means of numerical analysis and mathematical modeling. Modern high performance facilities allow solving the most resource intensive problems of computational science and engineering. Certainly one of the first places among them belongs to detailed numerical modeling of the non-stationary reactive flows and particularly the combustion phenomena in gaseous media. Most complex problems of combustion physics are related with evolution of the non-stationary and transient combustion regimes, which could be observed inside combustors of real technical and experimental facilities filled with highly reactive gaseous mixtures. Detailed analysis of these regimes features and peculiarities, identification of fundamental physical mechanisms and processes responsible for their dynamics and evolution is crucial for safety issues and developing novel propulsion devices and power stations, utilizing traditional or alternative energy sources more efficiently and environmentally safe. Due to the vast variety of factors and scales related to non-stationary gaseous combustion its theoretical and experimental analysis is limited to certain extent. And computational methods become the most insightful and powerful technique for combustion problems. Since the gaseous combustion process is highly sensitive to the adequacy of gas dynamic flow features reproduction, correct resolution of energy release zones and chemical transformations, results of modeling procedure are fully determined by the features of utilized computational method. Despite large variety of computational methods for modeling gas dynamic processes the problem of choosing the method appropriate for detailed combustion modeling is still
controversial. Only some of developed computational algorithms are capable for simulating
gas dynamic flows in compressible multicomponent mixtures of non-calorically perfect gases
with varying thermodynamic properties and in presence of energy release induced by chemical
transformations. Available computational resources make it possible to perform direct numerical
simulations of combustion processes inside multidimensional chambers utilizing advanced
physical models supplemented with detailed chemical kinetic schemes and taking into account
real features of flammable media and variety of processes accompanying combustion. However
despite continuous progress in increasing computational performance detailed numerical analysis
of non-stationary combustion processes inside vessels of technical or laboratory scales remains
very resource intensive task. Thereby numerical efficiency of the chosen numerical method
is of great importance on a par with accuracy and robustness. Today two main approaches
are commonly used to justify choice of numerical algorithm. First approach focuses on
accuracy order of the numerical method. Most common examples are weighted essentially
non-oscillating (WENO) finite difference and finite volume schemes and discontinuous Galerkin
(DG) methods with high accuracy orders [1]. Being wide spread and repeatedly used for various
problems of combustion phenomena modeling [2, 3, 4] these schemes have certain disadvantages.
WENO schemes have wide spatial stencils increasing with accuracy order that determines large
computational costs of WENO procedures and amount of interprocessor communication data
required for performing parallel computations. DG methods are computationally demanding
and tend to drop accuracy order so specific non-physical limiting procedures requiring user-
defined parameters are needed to maintain high levels of accuracy. Described drawbacks could
have major ineligible impact both on computational costs and obtained results accuracy crucial
for non-stationary combustion detailed modeling on large spatial and temporal scales. Second
approach that may be more perspective in a field of detailed combustion modeling consists in
developing low-order dissipative-free computational methods. A vivid example of computational
approach developed in a given ideology is CABARET method.

CABARET originates from work by Iserles on generalization of classical leapfrog numerical
method for solving hyperbolic equations. In [5] Iserles proposed upwind leapfrog scheme with
two-point spatial stencil and time discretization by the midpoint rule. It was also shown that
upwind leapfrog scheme is conditionally stable for Courant number within [0,1] interval. Further
detailed analysis of this scheme was performed in [6, 7], where it was called CABARET scheme
with considering its antisymmetrical spatial stencil. Main advantages of CABARET scheme are
compact spatial stencil, reversibility in time and capacity to provide exact solution with two
different Courant numbers 1 and 0.5. These properties determine outstanding dissipative and
dispersion features of the CABARET scheme [7]. Balance-characteristic CABARET version for
numerical solution of the one-dimensional gasdynamics equations was elaborated in [8]. Proposed
method with using flux variables correction necessary for providing monotonic solution has shown
high accuracy on classical blast wave benchmark problem [9]. Further it was shown that scheme
developed in [8] in case of special approximation of the initial conditions is monotonic [10] and
strongly monotonic [11] for Courant numbers within (0,0.5) and non-monotonic for Courant
numbers within (0.5,1). To avoid non-monotonic behavior two-step flux variables correction
procedure was developed in [10] that ensures monotonic solution by means of CABARET scheme
within entire stability region of Courant numbers in (0,1] interval. Lately two layer in time form
of the CABARET scheme [12, 13] became widely used for solving multidimensional problems
of gasdynamic [14] and hydraulic [15] flows. Monotonicity of this approach for one-dimensional
and two-dimensional cases was studied in [16, 17].

CABARET method has a number of outstanding features among which absolute absence of
numerical viscosity, most compact computational stencil, no need of any task specific parameters
or physically precarious limiting procedures [13]. However CABARET method was not yet
thoroughly tested in a field of multicomponent reactive flows modeling. This paper is devoted
2. Mathematical model and CABARET numerical procedure
2.1. Mathematical model
To perform numerical simulation of multidimensional flame dynamics in chemically active gaseous mixture full system consisting of mass, momentum and energy conservation laws for viscous, compressible multicomponent gasdynamics was solved, taking into account effects of thermal conductivity, molecular diffusion, chemical transformations and heat release and equations of state of real gas for each mixture component. Fuel-oxidizer chemical reactions were defined by detailed chemical kinetics mechanism. Full set of governing equations in divergence form are presented below:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = \sum_k M_k \left[ \frac{\partial}{\partial x_i} \left( \rho D_k(T) \frac{\partial Y_k}{\partial x_i} \right) \right]
\]

\[
\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial (\rho u_i Y_k)}{\partial x_i} = \left[ \frac{\partial}{\partial x_i} \left( \rho D_k(T) \frac{\partial Y_k}{\partial x_i} \right) \right] + \left( \frac{\partial Y_k}{\partial t} \right)_{chem}
\]

\[
\frac{\partial (\rho u_j)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_i} = \left[ \frac{\partial}{\partial x_i} \left( \sigma_{ji} - \delta_{ij} p \right) \right]
\]

\[
\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho u_i E)}{\partial x_i} = \left[ \frac{\partial}{\partial x_i} \left( u_j \sigma_{ji} - u_j \rho \right) \right] + \frac{\partial}{\partial x_i} \left( \kappa(T) \frac{\partial T}{\partial x_i} \right) + \sum_k h_k \left( \frac{\partial Y_k}{\partial t} \right)_{chem}
\]

Where viscous stress tensor

\[
\sigma_{ij} = \mu(T) \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \mu(T) \frac{\partial u_m}{\partial x_m}
\]

System is enclosed with following real gas equations of state:

\[
p = RT n = RT \sum_k Y_k
\]

\[
\varepsilon = c_V(T) T / \rho
\]

Here \( x_i \) - spatial coordinates, \( p, \rho, u_i \) - pressure, density and components of mass velocity vector, \( Y_k \) - molar concentration of \( k \)-th species, \( M_k \) - molar mass of \( k \)-th species, \( n = \sum_k Y_k \)

\( E = \varepsilon + u^2/2 \) - specific total energy, \( \varepsilon \) - specific inner energy, \( R \) - universal gas constant, \( \sigma_{ij} \) - the viscous stress tensor, \( c_V = \sum_k c_{V_k} Y_k \) - mixture constant volume volumetric heat capacity, \( c_{V_k} \) - the constant volume molar heat capacity of \( k \)-th species, \( h_k \) - the enthalpy of formation of \( k \)-th specie, \( k(T) \), \( \mu(T) \) - thermal conductivity and viscosity coefficients, \( D_k(T) \) - diffusion coefficients of \( k \)-th specie, \( (\partial Y_k/\partial t)_{chem} \) - variation of \( k \)-th specie concentration due to chemical reactions. Temperature dependence of the specific heats, heat capacities and enthalpies of each species were evaluated by interpolation of thermophysical JANAF data tables with fifth order polynomials [18]. The transport coefficients were calculated from the first principles of the gas
kinetic theory [19]. Variations of mixture components concentrations in chemical reactions were defined by the solution of the ordinary differential equations system

$$\frac{dY_k}{dt} = F_k (Y_1, Y_2, Y_3, ..., Y_N, T), \quad k = 1, \ldots, N$$

The right hand parts of equation system contain the rates of chemical reactions, which depend on temperature according with Arrhenius law in a standard form [20].

2.2. CABARET numerical procedure
Detailed description of CABARET numerical algorithm can be found in monograph by Goloviznin et al. [13]. Here we provide general expressions of CABARET procedure for the system of governing equations described above. The initial governing system, excluding equations for component transfer, can be rewritten in simpler form:

$$\partial \vec{\varphi} \partial t + A_i \partial \vec{\varphi} \partial x_i = 0$$

Where \( \vec{\varphi}^T = (\rho, u_i, p) \)

Being of balance-characteristic type, CABARET numerical method requires derivation of the governing equations system in characteristic form. In general characteristic form can be written as follows:

$$\left( \Omega_i \cdot \frac{\partial \vec{\varphi}}{\partial t} \right) + A_i \cdot \left( \Omega_i \cdot \frac{\partial \vec{\varphi}}{\partial x_i} \right) = \Omega_i \cdot \vec{f} - \Omega_i \sum_{j \neq i} A_j \frac{\partial \vec{\varphi}}{\partial x_j}$$

Where in our case

$$\vec{f}^T = \left( F_\rho, \frac{F_{u_i} - u_i F_\rho}{\rho}, \frac{1}{\rho} \frac{\partial p}{\partial x_i} \left( F_E + \left( u_i^2 - E \right) F_\rho - u_i F_{u_i} \right) + \frac{\partial p}{\partial \rho} F_\rho \right)$$

\( \Omega_i \) matrix composed from left eigenvectors of matrix \( A_i \), \( \Lambda_i = E \cdot \lambda_i \), where \( E \) unity matrix and \( \lambda_i \) eigenvalues vector of matrix \( A_i \).

$$F_\rho = \sum_k M_k \left[ \frac{\partial}{\partial x_i} \left( \rho D_k (T) \frac{\partial Y_k}{\partial x_i} \right) \right]$$

$$F_{u_i} = \left[ \frac{\partial}{\partial x_i} \left( u_j \sigma_{ji} \right) \right]$$

$$F_E = \left[ \frac{\partial}{\partial x_i} \left( u_j \sigma_{ji} \right) + \frac{\partial}{\partial x_i} \left( \kappa (T) \frac{\partial T}{\partial x_i} \right) \right] + \sum_k h_k \left( \frac{\partial Y_k}{\partial t} \right)_{chem}$$

Utilization of characteristic form of the governing equations system determines accurate localization of the solution features as shock waves and contact surfaces. At once approximation of the divergence form of the governing equation system performed during CABARET procedure ensures conservativity of the obtained solution.

Considering real equation of state pressure derivatives are obtained:

$$\frac{\partial p}{\partial \rho} = c^2 - \frac{(\gamma - 1) p}{\rho}, \quad \frac{\partial p}{\partial e} = (\gamma - 1) \rho$$

Required adiabatic index and speed of sound for multicomponent mixture were found as follows:

$$\gamma = 1 + \frac{n R}{c v}, \quad c = \sqrt{\gamma P / \rho}$$

To avoid negative values of species concentrations and preserve solution monotonicity convective species transport is obtained by using mass flow through cells faces calculated as a result of CABARET procedure.
3. Non-stationary combustion processes

3.1. Laminar flames test problem

Developed approach to numerical modeling via CABARET method was tested on one-dimensional stationary laminar flame propagation problem. In absence of multidimensional factors flame ignited near closed end of channel filled with combustible mixture after passing through short transient stage proceeds in stable stationary regime characterized by laminar flame velocity which is defined merely by the features of chemical kinetics and background flow induced by transient flame ignition processes. Convergence properties of the problem solution with decreasing computational cell size provide an insight about accuracy of the flow reproduction provided by numerical method. Results of convergence test on laminar flame propagation problem in stoichiometric hydrogen-oxygen mixture are given on figure 1. Dependence of laminar flame velocity and flame front thickness on computational cell size obtained using CABARET method is shown on figure 1 together with results obtained with classic euler-lagrange gasdynamic computational method known as coarse particles method (CPM) [21]. Earlier CPM was intensively used by authors for solving various problems of combustion physics and demonstrated high stability and effectiveness [22, 23]. The major drawback of CPM is high artificial diffusion that can introduce some undesirable features of obtained results. Negative effect of numerical diffusion arising while solving laminar flame propagation problem appears in a lower rate of solution convergence. As seen from figure 1 CPM solution converges about four times slower than solution provided by CABARET. Figure 2 shows clearly wider reaction zone for CPM solution on the same cell size, although flame structure obtained by both CABARET and CPM is qualitatively similar that indicates correctness of developed CABARET technique implementation.

3.2. Confined flames evolution

In present research we were mainly focused on features of the flame evolution inside confined chambers. Problem of confined flames evolution which is very important from the point of view of numerous practical applications is still far from general theoretical description. Non-stationary confined flame evolution is defined by effects of development of multidimensional flame surface instabilities, intensive interactions between flame surface and flame induced acoustics and swirling flows, peculiarities of chemical kinetics and thermophysical properties of combustible mixture at abrupt conditions changes posed by presence of shock waves and...
tangent discontinuities. Gasdynamical nature of the most of the outlined effects indicates crucial importance of precise reproduction of gasydynamic flows by numerical algorithm. Gasdynamical benchmark tests performed by authors of CABARET method have shown outstanding efficiency and accuracy for long-term calculations of acoustic and vortex flows. These positive properties of CABARET method are evident while solving problem of flame propagation out from the ignition source inside closed channel.

First consider rectangular channel filled with stoichiometric hydrogen-oxygen mixture. Mixture is being ignited near the left channel end-wall by cylindrical heated region that resembles energy release by spark plug induced gas breakdown. Primal ignition area surface is slightly disturbed to create ignition conditions more similar to real experimental ones. Experimental investigations of confined flames ignition in wide tubes shows that flame propagation out from the ignition source is almost isotropic and the longitudinal propagation velocity is almost the same as transverse up to the very moment of flame achieving channel side walls. However this behavior is rarely reproduced numerically even with utilization of high order numerical schemes [24].

Flame expansion out from the ignition source can be divided into several stages. On the initial stage immediately after ignition flame propagates as freely expanding cylindrical flame, without any effect of confinement. Duration of flame propagation in this regime is restricted by the distance between flame surface and channel walls as the ignition and flame non-stationary flame expansion propagation induce acoustic waves that propagate with sonic speed in the fresh mixture, reflect from the channel walls and interact with the flame surface providing repelling effect. While flame is approaching channel walls interaction between flame and acoustics becomes more violent and other counteractive process is required to maintain spherical expansion. Expanding flame is subjected to various hydrodynamic instabilities with finite characteristic time scales required for their development. Development of hydrodynamic instabilities on the flame front results in local multidimensional strain and wrinkling of the flame front surface. Due to the flame curvature eddies are generated in the vicinity of the flame surface. On the initial stage of flame expansion eddies are growing while diffusing into combustion products area. As the flame advances near the channel walls counterflow starts to slow down flame front propagation and eddies could manage to penetrate into fresh mixture ahead of the flame due to diffusion and cause intense mixing and enhance flame propagation velocity.

However characteristic time is needed for instabilities to start having a noticeable impact on flame dynamics. Let us consider relatively narrow channel of 5 mm width. Results obtained with CABARET and CPM methods on the same time instance corresponding to flame surface achievement channel side walls via CABARET method are presented on figure 3. Here
CABARET and CPM provide almost similar results that indicate that both methods reproduce interactions between acoustic waves and flame front contact discontinuity almost identically. Narrow channel width significantly limits duration of initial freely cylindrical flame propagation and instabilities development at this stage. Not being able to grow significantly flame surface instabilities are damped by intense acoustics reflected from the side walls. Thereby in narrow channel notable anisotropic expansion is observed with much stronger longitudinal compared with transverse flame surface strain. Situation drastically changes in wider channel of 2 m width results for which are presented in figure 4. Here we observe pronounced instability growth on the flame surface that results in faster transverse flame propagation and isotropic flame expansion in case of CABARET in comparison with CPM. Rugged flame front surface represent so called cellular flame structure that is more pronounced due to developed flame surface instability in CABARET solution. Examining flow structure near flame surface (figure 5) one could notice intensive vorticity of the flow in CABARET solution while vortex formation in CPM solution is suppressed by higher numerical diffusion (figure 6).

Described phenomenon may be crucial for detailed analysis of combustion wave acceleration process proceeding after flame ignition in semi-closed tubes. More pronounced transversal flame propagation restricts possible extension of the flame surface while adopting to the structure of the background flow [25, 26]. Gasdynamical flame acceleration after a certain time instance becomes caused by interaction between flame skirt and vortices generated in boundary layer behind leading shock wave (figure 7). However as it was shown in [27] flame acceleration due to gasdynamical factors cannot be a key mechanism on final stages of deflagration-to-detonation transition process since the restriction imposed on gasdynamical acceleration by Vulis law of inverse action [28]. Thus the interaction between flame front and vortices generated in boundary layer can be important only until flame front achieves velocities in laboratory reference system equal to sonic speed in combustion products. On the other hand obtained flame front flattening due to more accurate reproduction of flame interactions with acoustic waves and vortex generation may be essential for theoretical foundation of the tulip flame structure formation in opened tubes that was observed in recent experiments [29].
Figure 7. Flame front acceleration process in a smooth tube. Vortices diffusion from boundary layer starts to play significant role on the flame dynamics after a certain time period from ignition.

4. Conclusions
Accurate simulation of gasdynamic processes accompanying flame propagation in gaseous mixtures is crucial for correct interpretation of underlying physical mechanisms therefore low-order dissipation-free methods like CABARET method seem to have high potential for reliable simulation of complex combustion physics phenomena. Obtained results have shown that diminishing artificial viscosity makes it possible to use rougher computational grids without serious loss of precision of reproducing key features of developing flow structures. Solution of non-stationary combustion evolution out from the ignition source in rectangular channel by means of CABARET technique allowed to obtain results similar to that observed in real experiments and to justify the difference occurring while using classical coarse particles method by more accurate modeling of flame surface instabilities end flame induced acoustics provided by CABARET method. Utilization of CABARET method also allowed to analyze possible influence of flame interaction with flow vorticity generated in boundary layer on flame acceleration process that could have strong quantitative effect on flame acceleration in channel.

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