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# Role of numerical scheme choice on the results of mathematical modeling of combustion and detonation

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**Abstract.** The present study discusses capabilities of dissipation-free CABARET numerical method application to unsteady reactive gasdynamic flows modeling. In framework of present research the method was adopted for reactive flows governed by real gas equation of state and applied for several typical problems of unsteady gas dynamics and combustion modeling such as ignition and detonation initiation by localized energy sources. Solutions were thoroughly analyzed and compared with that derived by using of the modified Euler–Lagrange method of “coarse” particles. Obtained results allowed us to distinguish range of phenomena where artificial effects of numerical approach may counterfeit their physical nature and to develop guidelines for numerical approach selection appropriate for unsteady reactive gasdynamic flows numerical modeling.

## 1. Introduction

Numerical modeling is one of the most effective techniques for theoretical analysis of fundamental and applied problems of combustion and detonation physics. Increasing performance of modern computational facilities continuously expands the range of problems that could be solved by means of numerical methods. However the problem of choosing a proper numerical approach for modeling the process of unsteady reactive gasdynamic flows evolution on the long time periods and on precise three-dimensional numerical grids is still controversial. First of all numerical method should be valid and properly resolve features of unsteady flows. No less important is the fact that the scales of real power and propulsion systems or laboratory facilities are ranging from several centimeters to several meters. To resolve gasdynamics of the combustion within such systems relatively coarse computational grids with cells up to several millimeters are sufficient. However combustion process is mainly defined by energy release in the reaction zone that is about fractions of millimeter for most of hydrocarbon-air mixtures. Thus the amount of computational cells for typical problems of unsteady combustion dynamics ranges up to several millions of cells. Taking into account the necessity of using detailed chemical kinetics schemes for proper resolution of the flame dynamics features [1] one can conclude that combustion modeling is by far one of the most computationally consuming problem and suitable method algorithm should be computationally effective and parallelizable.

Today it is common to justify numerical approach selection on the basis of its accuracy order. Unlike low order schemes, high order accurate schemes with suitable limiting procedures are almost deprived of artificial viscosity and can provide high resolution of studying processes on relatively rude computational grids. However implementation of high order schemes for



unsteady gasdynamic problems is hindered for several reasons. First, necessity of using large stencils complicates code parallelization and places additional computational and data exchange costs when using cluster supercomputers with distributed memory. Besides, reliability of high order accuracy schemes depends on the choice of limiting procedures and subgrid models that are different for each particular problem [2–7] and even for distinct stages of the unsteady process. Thus in a series of numerical experiments on flame acceleration process in confined channels [1] it was shown that flame front thickness varies as the flame passes through the channel and wherein the physical mechanisms defining flame propagation are altering either. Inaccurate choosing of correction procedures on each stage of the flame acceleration process can deceive thickness of the flame front and leading shock wave that may result in artificial coupling of the flame front and shock leading to premature deflagration to detonation transition and shortening run up distance (see e.g. [8] where the mentioned mechanism of detonation onset in the obstructed channel takes place contradicting with experimental criterion defining the origins of detonation via the shock reflection from the obstacle surface known as Thomas criterion [9]).

The second less widely spread option is utilization of low order accurate schemes developed in such a way that artificial viscosity, diffusion and dispersion impacts are minimized. Dissipation-free CABARET method is a representative of this class of numerical schemes. It was fully developed and described in series of papers by Goloviznin et al [10, 11]. CABARET method belongs to Godunov-type numerical method and possesses several unique features such as:

- the most compact computational stencil;
- second order accuracy in space and time in problems with flows not requiring flow correction procedure;
- physical flow correction procedure based on direct usage of maximum principle for local Riemann invariants;
- possibility for acoustic waves propagation modeling against the background of strongly non-uniform in space and time flows;
- numerical scheme does not cause attenuation or destruction of stationary vortexes, for propagating vortexes scheme dissipation effects are negligibly small;
- numerical scheme is explicit and does not require any iterative procedures;
- in number of cases absolutely dissipative-free and always has least approximal dispersion.

The most disadvantage of CABARET scheme is operation with extended set of flow parameters separated into two categories: “conservative” variables defined on cells centers and “flow” variables defined on cells faces. It imposes tight restrictions on computer random access memory capacities required for modeling via CABARET method. However resources of modern computational facilities easily meet these requirements. Abovementioned characteristics of the CABARET method stipulate the interest in possibilities of its appliance for solving unsteady reactive gasdynamic problems.

In addition to choosing the numerical procedure it is necessary to elaborate set of measures for its adequate testing on the basis of recent numerical experience in non-steady combustion and detonation modeling and obtained results interpreting. According to our recent experience in modeling the flame propagation inside closed vessels [1] and two-phase mixtures [12], the phenomenon of deflagration-to-detonation transition [13], the non-steady thermal explosion [14], the ignition by the transient sources of energy [15] etc. it was concluded that the following validation information is of prior interest:

- what is the effect of numerical dissipation on reacting sub- and supersonic flow evolution including the flame evolution;

- how adequate the chosen numerical procedure reproduces the peculiarities of transient regimes involving the reaction front propagation and its interaction with acoustic fields and compression waves;
- what is the influence on the critical phenomena evolution and as a result on the energy and geometry limits of the combustion regimes.

The aim of this paper was to define the basic problems of non-steady combustion and detonation physics and to implement and apply CABARET method for their solution. The paper is organized as follows. Section 2 is devoted to the benchmark problem setups formulation. In section 3 the governing equation system and corresponding implementation of CABARET method are given. Section 4 represents the validation of CABARET numerical method on the proposed test problems and the comparison between results provided by CABARET scheme and Euler-Lagrange “coarse particles” method extensively used by authors in their previous research devoted to numerical investigation of nonstationary flame propagation processes in pure gaseous combustible mixtures and mixtures with suspended microparticles [16,17]. We conclude in section 5 devoted to the discussion of specific problems of combustion and detonation physics where features of CABARET method may greatly influence correctness of provided results.

## 2. Benchmark tests formulation

For qualitative analysis of the reliability of the chosen numerical procedure for non-steady combustion phenomena representation it is sufficient to consider one-dimensional problems related with different aspects of the reacting flow evolution due to the energy release inside the reaction zone. According to the basic aspects of method validation formulated in the introductory section it seems to be useful to consider the following one-dimensional problems. First of all it is quite important to reproduce accurately the sub- and supersonic flows and to understand the effects of artificial numerical factors on the contact surfaces and compression waves stability in both cases. It is known that the flame is able to accelerate inside the closed vessels (channels) and it is necessary to reproduce adequately the interactions between the flame and the emerging flow structures. Second it is crucial to reproduce the flame structure itself at different ambient conditions. Third it is essential to consider the non-steady processes involving the flame acceleration and interaction with contact surfaces and compression waves. To solve the later problem it is useful to consider a classical Zel'dovich problem of non-steady thermal explosion on the background of reactivity gradient [18]. There is a set of solutions of this problem [14, 18] including the formation of sub-sonic reaction wave, propagating in the flow behind the shock wave, reaction wave propagating with acceleration and transforming into the detonation and detonation formation via the coupling of supersonic reaction front and the shock wave. Thus the solution of such a basic problem should provide useful information on the adequacy of chosen numerical procedure for reproduction of non-steady combustion processes in a wide range of ambient conditions. The fourth problem seemed to be of importance is the reproduction of critical conditions for different combustion regimes. It is known that the direct detonation initiation can be caused only by the sufficient energy sources. Furthermore there is an experimentally reproduced peculiarity in the vicinity of energy limit of detonation initiation. At near-limit energy the detonation arises via transient process involving the reaction front acceleration and its transformation first into the overdriven detonation wave and then into the steady self-sustained detonation [15, 19]. Obtaining reliable critical energy input values is of paramount interest per se and besides can serve as an additional argument in favor of choosing of the numerical approach most suitable for solving problems of combustion and detonation physics.

All of the problem setups are considered for stoichiometric hydrogen–oxygen mixture at normal ambient conditions as its combustion kinetics is the best known for today and adequate experimental data on the combustion parameters is available for verification.

### 2.1. Subsonic and supersonic flows

To reproduce numerically a subsonic or supersonic flow one can solve a problem of discontinuity decay. Depending on the pressure drop a driver gas flows into the driven gas in sub- or supersonic regime. In such a case a contact discontinuity follows the mean flow with the constant velocity. The steady solution implies the constancy of contact surface thickness and propagation speed. Any deviations in absence of physical diffusivity should be interpreted as a numerical artifact.

Let consider the subsonic flow in the system where the air compressed up to 2.0 atm flows into the air at normal conditions (at pressure 1.0 atm). The gas in such conditions flows with the velocity of 87 m/s. The supersonic flow will be considered in the system where the hydrogen compressed up to 20.0 atm flows into the air at normal conditions. The gas in such conditions flows with the velocity of 720.0 m/s. The evolutions of contact surface and flow parameters are the main output data of this test.

### 2.2. Steady flame propagation

The steady flame propagation regime can be observed inside the semi-opened channel after the ignition near the closed end-wall by low-energy source. After a transient stage a steady flame forms which propagates along the channel walls with constant speed determined by the energy release inside the flame front and combustion products expansion in the gap between the end-wall and the flame front. The speed value can be estimated as a composition of burning velocity  $U_f$  and expansion factor  $\Theta$  calculated as densities ratio  $\rho_f/\rho_b$ , where  $\rho_f$  is the density of the fresh mixture and  $\rho_b$  is the density of the combustion products:

$$U_{f,lab} = \Theta U_f. \quad (1)$$

According to this a normal flame velocity (burning velocity) can be obtained numerically knowing the one-dimensional solution for  $U_{f,lab}$  and  $\Theta$ . Besides the burning velocity can be obtained via the full integration along the flame front as [20]:

$$U_f = \frac{\int_{L_f} \dot{Y}_i dl}{Y_{ia} - Y_{ib}} \frac{1}{\rho}. \quad (2)$$

The problem setup for this test can be formulated as follows. The flame is initiated by the heated planar layer of given thickness (1.0 mm) and temperature (3000.0 K) in the vicinity of the end-wall. The output data are evolutions of flame front parameters such as  $U_{f,lab}$ ,  $U_f$ ,  $\Theta$  and flame thickness  $L_f = (T_b - T_a)/\max|\text{grad } T|$ . As the non-steady flame propagates at permanently changing ambient conditions it is of interest to verify the temperature and composition dependencies of the burning velocity comparing the calculations with available experimental data.

### 2.3. Non-steady reaction waves within thermal explosion

Let us follow the classical problem setup proposed by Zel'dovich [14,18] and consider the linear temperature non-uniformity with maximal temperature value ( $T^*$ ) sufficient for auto-ignition (e.g. 1500.0 K):

$$T(x) = \begin{cases} T^* - (T^* - T_0)x/L, & \text{if } x < L, \\ T_0, & \text{if } x \geq L, \end{cases} \quad (3)$$

where  $T_0$  is the ambient temperature (300.0 K),  $L$  is the linear scale (length) of the temperature gradient. According to the Zel'dovich concept independent ignitions along the reactivity gradient can be represented as a spontaneous wave propagating with a characteristic speed estimated as:

$$U_{sp} = |\text{grad } \tau_{ind}|^{-1}, \quad (4)$$

which in our case can be written as:

$$U_{sp} = \left( \frac{d\tau_{ind}}{dx} \right)^{-1} = \left( \frac{d\tau_{ind}}{dT} \frac{dT}{dx} \right)^{-1} = \left( \frac{d\tau_{ind}}{dT} \frac{T^* - T_0}{L} \right)^{-1}, \quad (5)$$

where  $\tau_{ind}$  is induction period of the reaction which in general case is a function of temperature, pressure and mixture composition and is determined by the kinetic mechanism of gaseous mixture combustion. The different regimes of ignition and sequential combustion propagation can be obtained varying the gradient length  $L$ . According to Zel'dovich classification the small  $L$  corresponds to slow combustion waves formation while the large  $L$  corresponds to high speed combustion waves such as detonation, weak detonation and finally as a steady thermal explosion (in case of infinite value of  $L$ ). Recently [14] a wider classification of the regimes on the example of hydrogen-containing mixtures was obtained. On the basis of these results it seems to be useful to consider the influence of numerical effects on the different non-steady solutions while using different numerical procedures. The output data should contain the integral diagram representing the limits of different regimes depending on the gradient length  $L$ .

#### 2.4. Regimes of direct detonation initiation

The problem setup for the direct detonation initiation test is close to that accepted for steady flame test. The difference is in the way of energy input. To initiate detonation a sufficiently higher energy is needed than for a regular ignition. Here we propose to initiate the detonation by the  $0.1 \mu s$  energy pulse localized in the planar layer of given thickness (1.0 mm) in the vicinity of the end-wall. For simplicity it is convenient to use energy input linear in time as was accepted in [15]. As it was mentioned above depending on the energy value different regimes are possible: (i) direct detonation formation behind the strong shock emerging on the margin between the fresh mixture and hot layer, (ii) detonation formation via transient process involving reaction front formation, its acceleration in the flow behind the outrunning shock and transformation into the detonation and (iii) high speed reaction front formation with its sequential deceleration. The output data in case of this test should contain the information about the energy limits between the described regimes.

### 3. Mathematical model

All abovementioned benchmarks were carried out solving the onedimensional, time-dependent, reactive gas dynamics equations including the effects of gas compression, molecular diffusion, thermal conduction and detailed chemical kinetics scheme for hydrogen oxidation. Equations system was supplemented with tabular equation of state.

#### 3.1. Governing equations

Governing equations system has the following form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \quad (6)$$

$$\frac{\partial Y_i}{\partial t} + \frac{\partial (Y_i u)}{\partial x} = \frac{1}{\rho} \frac{\partial}{\partial x} \left( \rho D_i(T) \frac{\partial Y_i}{\partial x} \right) + \left( \frac{\partial Y_i}{\partial t} \right)_{chem}, \quad (7)$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2)}{\partial x} = - \frac{\partial P}{\partial x}, \quad (8)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E u)}{\partial x} = - \frac{\partial (P u)}{\partial x} + \frac{\partial}{\partial x} \left( \kappa(T) \frac{\partial T}{\partial x} \right) + \sum_k h_k \left( \frac{dY_k}{dt} \right), \quad (9)$$

$$P = R_B T n, \quad (10)$$

$$\varepsilon = c_v T / \rho. \quad (11)$$

Here  $P$ ,  $\rho$ ,  $u$  are the pressure, density and mass velocity,  $Y_i$  is the molar concentration of  $i$ -species,  $E = \varepsilon + u^2/2$  is the specific total energy,  $\varepsilon$  is the specific internal energy,  $R_B$  is the universal gas constant,  $n = \sum_i Y_i$  is the mixture molar density,  $\sigma_{ij}$  is the viscous stress tensor,  $c_v = \sum_i c_{v_i} Y_i$  is the mixture constant volume volumetric heat capacity,  $c_{v_i}$  is the constant volume molar heat capacity of  $i$ -species,  $h_i$  is the enthalpy of formation of  $i$ -species,  $\kappa(T)$  and  $\mu(T)$  are the coefficients of thermal conductivity and viscosity,  $D_i(T)$  is the diffusion coefficients of  $i$ -species,  $(\partial Y_i / \partial t)_{\text{chem}}$  is the variation of  $i$ -species concentration (mass fraction) in chemical reactions.

The gas equation of state was taken with the temperature dependence of the specific heats, heat capacities and enthalpies of each species in accordance with the JANAF tables and interpolated by the fifth-order polynomials [21]. The transport coefficients were calculated from the first principles using the gas kinetic theory [22]. Concentrations of the mixture components  $Y_i$  are defined by the solution of chemical kinetics equations system

$$\frac{dY_i}{dt} = F_i(Y_1, Y_2, Y_3, \dots, Y_N, T), \quad i = 1, \dots, N. \quad (12)$$

The right hand parts of equation (12) contain the rates of chemical reactions, which depend on temperature according to the Arrhenius law in a standard form [21].

### 3.2. CABARET numerical procedure formulation

As governing equations system is of hyperbolic type, it can be cast to so-called characteristic form (for detailed procedure see e.g. [23]):

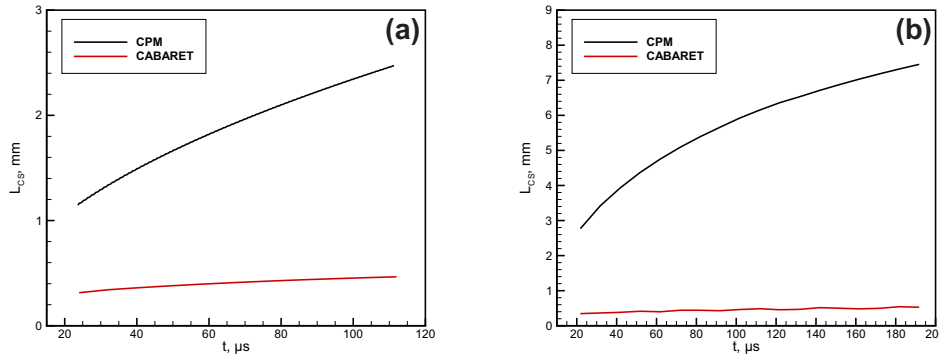
$$\left( \Omega \cdot \frac{\partial \vec{\varphi}}{\partial t} \right) + \Lambda \cdot \left( \Omega \cdot \frac{\partial \vec{\varphi}}{\partial x} \right) = \Omega \cdot \vec{f}, \quad (13)$$

where

$$\begin{aligned} \vec{\varphi}^T &= (Y_1, \dots, Y_N, \rho, u, P), \\ \vec{f}^T &= \left( Y_{1_{\text{prod}}}, \dots, Y_{N_{\text{prod}}}, 0.0, \frac{E_{\text{prod}}}{\rho} \frac{\partial P}{\partial \varepsilon} \right), \\ \Omega &= \begin{pmatrix} 0 & \dots & 0 & 0 & 1 & 1/\rho c \\ 0 & \dots & 0 & 0 & 1 & -1/\rho c \\ 0 & \dots & 0 & -c^2 & 0 & 1 \\ 1 & \dots & 0 & 0 & 0 & -Y_1/\rho c^2 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 1 & 0 & 0 & -Y_N/\rho c^2 \end{pmatrix}, \\ \Lambda &= \begin{pmatrix} u+c & 0 & 0 & 0 & \dots & 0 \\ 0 & u-c & 0 & 0 & \dots & 0 \\ 0 & 0 & u & 0 & \dots & 0 \\ 0 & 0 & 0 & u & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & u \end{pmatrix}. \end{aligned}$$

Here

$$Y_{i_{\text{prod}}} = \frac{1}{\rho} \frac{\partial}{\partial x} (\rho D_i(T) \frac{\partial Y_i}{\partial x}) + \left( \frac{\partial Y_i}{\partial t} \right)_{\text{chem}}$$



**Figure 1.** Contact surface width evolution: (a)—subsonic flow; (b)—supersonic flow.

is the source of  $i$ -th species due to diffusion and chemical reactions,

$$E_{\text{prod}} = \frac{\partial}{\partial x} \left( \kappa(T) \frac{\partial T}{\partial x} \right) + \sum_k h_k \left( \frac{dY_k}{dt} \right)$$

is the source of energy due to heat transfer, diffusion and chemical reactions.

The procedure for evaluation of speed of sound  $c$  in multicomponent mixture governed by equations of state (10) and (11) requires prior determining of adiabatic index. In present research adiabatic index was found as follows:  $\gamma = 1 + nR_B/c_v$  herewith speed of sound  $c = \sqrt{\gamma P/\rho}$ .

For solving governing equations (6)–(9) we adopted algorithm described by Goloviznin et. al [10,11,23] with considering derived characteristic form (13) and expression for speed of sound  $c$ . The solving procedure boils down to four main stages:

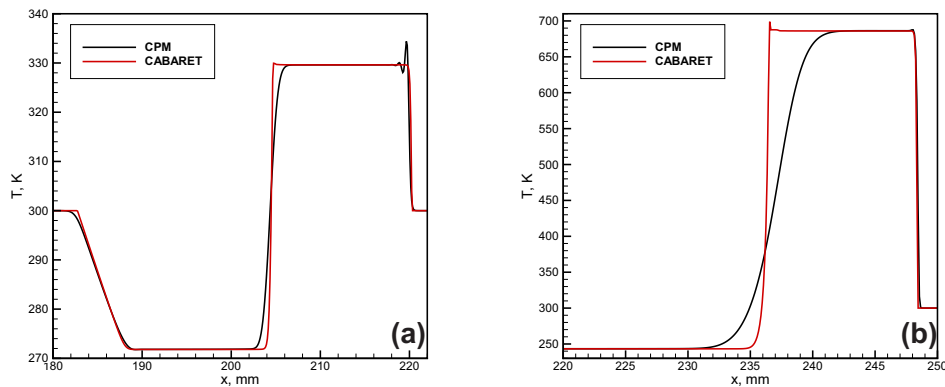
- (i) Conservative form (6)–(9) of governing equations is approximated by difference scheme of second order in time from which conservative variables on a half time step are derived.
- (ii) Intermediate half-step conservative variables and characteristic form (13) are used for local Riemann invariants (“quasi-invariants”) evaluation.
- (iii) Flow variables on computational cells bounds on the next time step are determined as a result of “quasi-invariants” transfer along characteristics.
- (iv) From the approximation of conservative form of governing equations system with second order implicit scheme conservative variables on the next time step are found. The calculation with the implicit scheme becomes possible as at this stage flow variables on the next time step are already known.

## 4. Benchmark tests results

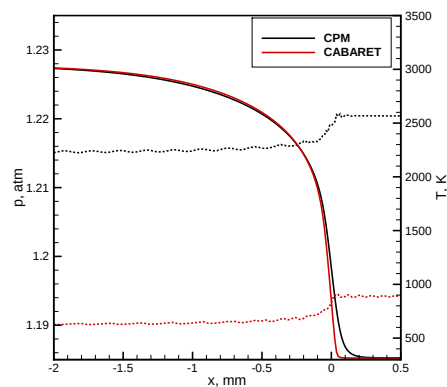
### 4.1. Subsonic and supersonic flows

Figure 1 represents the behavior of contact surfaces propagating in the sub- and supersonic flows according to the problem setups formulated in subsection 2.1. Figure 2 shows the characteristic flow structures in the vicinity of the contact surfaces in both cases. One can observe that relatively low numerical viscosity of CABARET scheme provides less artificial thickening of the contact surface propagating in the subsonic and supersonic flows (see figure 1a,b). Using both CABARET and CPM schemes one can observe a saturation of contact surface thickening. In case of choosing CPM scheme the effective velocity of contact surface thickening at the saturation level equals approximately 7.0 m/s. CABARET scheme provides almost no additional increase in contact surface thickness with time. It should be also noted that CABARET scheme

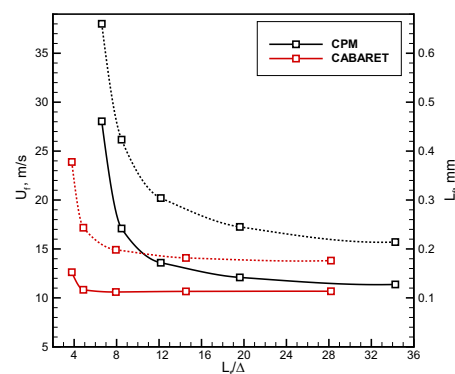




**Figure 2.** Temperature profiles: (a)—subsonic flow; (b)—supersonic flow.



**Figure 3.** Structure of the steady-state laminar flame. Solid lines denote temperature profile, dashed lines denote pressure profile.

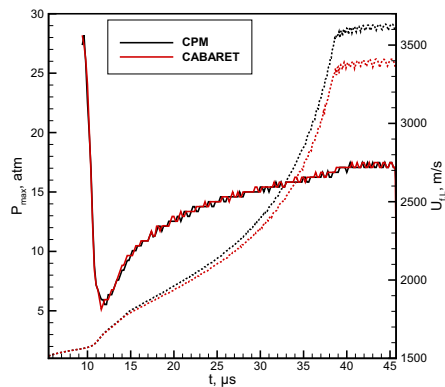


**Figure 4.** Resolution dependence of normal flame velocity (solid lines) and flame thickness (dashed lines).

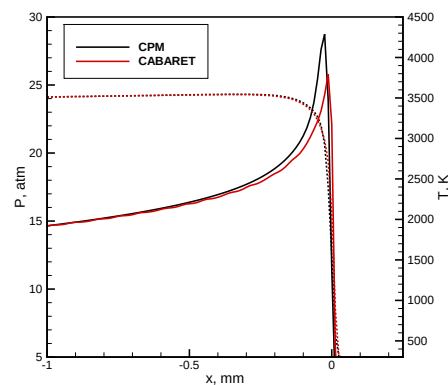
possesses less ( $\sim 3-4$  times) sensitivity towards the choice of numerical grid resolution that provides faster convergence of the solution. When studying supersonic flow according to the problem setup formulated in subsection 2.1 a sonic point is situated directly on the contact surface. The flow velocity in this case is 720.0 m/s, sonic speed in the compressed air is 520.0 m/s and in the expanding hydrogen is 1200.0 m/s. At the early transient stage of the process evolution perturbations arise in the vicinity of the contact surface which are not higher than  $3.0 \times 10^{-4}\%$  of the average values of temperature and pressure ahead the leading shock wave. These perturbations are negligible compare with those (0.2%) forming at the shock front while using CPM approach (see figure 2a). Moreover they are attenuating in time. Presented results allow highlighting the advantages of CABARET approach which are lower value of scheme diffusion and absence of artificial oscillations which despite their constancy are able to complicate sufficiently the analysis of calculations.

#### 4.2. Steady flame propagation

The results of steady flame tests are presented in figures 3 and 4. Figure 3 shows the temperature and pressure profiles in the vicinity of the flame front. One can observe close results obtained using two numerical schemes and the same numerical grid resolution. Figure 4 provides



**Figure 5.** Transient thermal explosion process evolution. Solid lines illustrate combustion wave velocity time history, dashed lines represent pressure change over time.



**Figure 6.** Stationary detonation wave structure. Solid lines denote pressure profiles, dashed lines are temperature profiles.

**Table 1.** Detonation wave parameters in Chapman–Jouguet point.

| Method  | $D_{CJ}$ (m/s) | $P_{CJ}$ (atm) | $T_{CJ}$ (K) | $c_{CJ}$ (m/s) | $M_{CJ}$ |
|---------|----------------|----------------|--------------|----------------|----------|
| CABARET | 2730.0         | 21.45          | 3388.4       | 1532.7         | 5.065    |
| CPM     | 2730.0         | 21.72          | 3451.2       | 1541.9         | 5.065    |

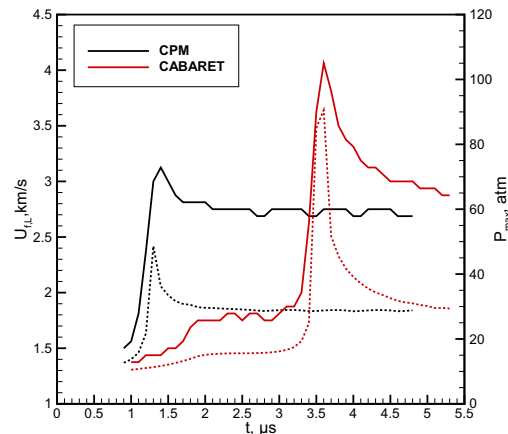
**Table 2.** Detonation wave parameters in von Neumann peak and critical detonation initiation energy.

| Method  | $u_{vN}$ (m/s) | $P_{vN}$ (atm) | $T_{vN}$ (K) | $c_{vN}$ (m/s) | $E_{cr}$ (kJ/m <sup>2</sup> ) |
|---------|----------------|----------------|--------------|----------------|-------------------------------|
| CABARET | 1942.9         | 26.17          | 2453.12      | 1388.54        | 7.2                           |
| CPM     | 2023.3         | 29.54          | 2899.18      | 1483.01        | 2.9                           |

information on the resolution dependence of the solution obtained using two schemes. Normal flame velocity obtained by both methods converges to  $\sim 10.6$  m/s that is in a good agreement with available computational and experimental data [24]. According to the obtained results one can conclude that the CABARET scheme possesses twice faster convergence and provides almost the same solution on twice ruder grid which is of great importance when solving complex multidimensional problems requiring large computational costs.

#### 4.3. Non-steady reaction waves within thermal explosion

Figure 5 reveals the solution for transient thermal explosion process. The temperature gradient length in the presented case is 8.0 cm that corresponds to the formation of self-sustained detonation wave via the transient process involving the reaction wave acceleration in the flow behind the out-running shock wave. Both numerical schemes provide almost the same solutions



**Figure 7.** Detonation initiation regimes by means of localized transient energy source. Solid lines denote combustion wave velocity evolution, dashed lines denote maximum pressure time history.

when using the same numerical grid resolution in the convergence range. The distinctions are mainly concerns the parameters of the von Neumann peak of the steady detonation wave. All the parameters of steady detonation wave are presented in tables 1 and 2 where also a critical detonation initiation energy is presented which will be discussed in the next subsection. The structure of self-sustained detonation propagating in the stoichiometric hydrogen–oxygen mixture is presented in figure 6.

#### 4.4. Regimes of direct detonation initiation

When studying the detonation formation as a result of spontaneous wave evolution on the background of temperature gradient (see previous subsection) the basic mechanism responsible for reaction front formation is chemical kinetics which determines sequential independent ignitions all over the initial temperature gradient. In case of detonation initiation by means of transient energy source localized in the relatively small spatial region the gasdynamics becomes to play a leading role. Due to this a numerical scheme with higher numerical viscosity (CPM) provides lower detonation initiation limit (see table 2). The evolutions of the process initiated by the  $7.2 \text{ kJ/m}^2$  source reproduced using two numerical schemes are presented in figure 7. In case of CPM approach a process evolves as following: a discontinuity decay taking place on the margin of energy input region produces a shock and a reaction front propagating from the margin behind the shock. Due to relatively thick reaction front and the shock compare with those reproduced by CABARET technique their coupling takes place in the very vicinity to the margin and one is not able to recognize a transient stage of the process evolution which is clearly seen in case of less diffusive CABARET scheme. Thus in case of studying the transient processes of combustion and detonation the choice of numerical scheme can provide qualitatively different solutions.

## 5. Conclusions

Considered computational tests illustrate the advantages of diffusion-less computational schemes compare with conventional Euler–Lagrangian techniques providing versatile information about the transient combustion and detonation phenomena. Physical flow correction procedures designed to diminish the numerical diffusivity effects allow to carry long-time calculations on at least twice lower numerical grid resolution with negligible influence of numerical artefacts.

Furthermore the diminishing of the numerical diffusivity can qualitatively change the solution for transient processes such as detonation onset due to the reaction front acceleration. According to the obtained results it seems to be prospective to utilize such numerical schemes (CABARET-like) to reproduce accurately the transient reactive flows including non-steady flames and detonations.

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