The objective of the study outlined in this paper was to develop the computationally efficient algorithm for multidimensional numerical simulation of deflagration-to-detonation transition (DDT) in gas-fueled air-breathing pulse detonation engine (PDE). It is implied that the availability of such an algorithm will allow for more realistic estimates of PDE performances (specific impulse, thrust, etc.) than those obtained with the presumption of direct detonation initiation. The new algorithm is based on the coupled Flame Tracking–Particle (FTP) method implemented into the standard computational fluid dynamics (CFD) code solving the Reynolds Averaged Navier–Stokes equations by the control-volume technique. The coupled methodology has been applied to the two-dimensional (2D) numerical simulation of DDT in a PDE channel 3 m long with flame accelerating obstacles and shock-wave focusing nozzle filled with the stoichiometric propane–air mixture at normal initial conditions. The fuel-based specific impulse was estimated as 2480 s.

1 INTRODUCTION

Realistic estimates of PDE performances (specific impulse, thrust, etc.) require consideration of DDT rather than direct detonation initiation in the PDE tube. Despite the DDT phenomenology is currently well understood [1], its adequate numerical simulation is still not possible. The reason is the necessity of resolving a wide spectrum of length and time scales inherent in the DDT phenomenon and therefore the need in extremely high CPU power.

The classic mechanism of DDT in a straight smooth tube includes several stages [2, 3], namely, (i) forced mixture ignition with the formation of a laminar flame; (ii) progressing increase in the rate of combustion because of the appearance of instabilities and subsequently turbulent flow ahead of the flame front; (iii) shock wave formation and strengthening ahead of the accelerating flame front; (iv) self-ignition of the shock-compressed mixture in the region between the shock wave and flame front [4] (“explosion in the explosion” [5]) resulting
in the formation of an overdriven detonation wave; and then (ν) self-sustaining Chapman–Jouguet (CJ) detonation. The time and distance of the DDT are known to be largely determined by the first three stages [6]. Deflagration-to-detonation transition in air mixtures of hydrocarbon fuels requires that the “visible” velocity of the turbulent flame front in the laboratory coordinate system be higher than 1000 m/s [7]. At such a flame front velocity, the shock wave running ahead has a velocity higher than 1300 m/s (the shock wave Mach number is $M \approx 3.8$), and the pressure and temperature of the explosive mixture behind it are higher than 1.7 MPa and 1200 K, respectively.

The mechanism of DDT in tubes with regular obstacles [3, 8] is in many respects similar to the mechanism [2–6] described above. There are also important differences. First, the flame is accelerated much more quickly in a tube with obstacles because of the additional turbulization of a fresh explosive mixture when it flows around obstacles. Second, there appear new possibilities for gas ignition. A gas can autoignite in the shock wave reflected from an obstacle or (if obstacles are large) because of mixing of directed jets of hot combustion products with a cold fresh explosive mixture.

At present, there exist few attempts of numerical simulation of DDT in gases. The most successful is seemingly one by Oran and Gamezo who published a series of papers on DDT in hydrogen–air mixtures in channels with regular obstacles [9, 10]. They solved both three-dimensional (3D) and 2D Navier–Stokes equations coupled with the energy conservation equation and the kinetic equation for the single-stage overall chemical reaction. Despite the results of [9, 10] revealed some salient features of flame acceleration in the obstructed channels, the model applied in [9, 10] cannot be used for quantitative predictions. This model does not make a difference between the chemical kinetics of combustion in the flame front and chemical kinetics of autoignition. As is known, the reactions in flame do not exhibit ignition delays as the reactive mixture is ignited due to heat and active species diffusion from the high-temperature reaction zone. At autoignition, neither heat nor active species are supplied from outside and therefore the initial increase of the reaction rate is significantly slower than in the flame and the main role is played by relatively slow chain origination reactions. The latter means that the reaction rate constant in the overall reaction mechanism describing pre-flame autoignition should be significantly lower than that describing the reaction in the flame front. As a result, the use of identical reaction rate constants for both pre-flame and flame reactions in [9, 10] can become a reason of significant overestimation of pre-flame reaction rates.

The objective of any combustion model is to provide correct values of mean reaction rates regardless the combustion mode in a turbulent reactive flow. The mean reaction rate can be obtained provided one knows the reaction kinetics and the local instantaneous fields of temperature and species concentrations. The development of reaction kinetics is the separate task which is independent of combustion modeling. The only relevant issue is the CPU time required
for calculating instantaneous reaction rates. This issue can be overcome by applying properly validated short overall reaction mechanisms and/or lookup tables. The local instantaneous fields of temperature and species concentrations are usually not known. Therefore, one has to replace this lacking information by a combustion model.

There exist many combustion models both for laminar and turbulent flows. If chemistry is fast as compared to mixing, the Eddy-Break-Up model can be used [11]. It is simple but has a limited range of validity. There is a whole class of statistical combustion models (based on the formalism of probability density functions) with probabilistic representation of turbulence and its interaction with chemistry [12]. Despite many attractive features, this approach is still not capable of operating with complex chemistry due to inadequate CPU requirements. Moreover, such approaches do not resolve different scales in the turbulent flow and their energy content. Instead, all scales are treated indifferently whereas their effect on combustion and flame is different. Nevertheless, these approaches look very promising for treating autoignition problems. The other class of models deals with a flamelet approach [13]. In this approach, the instantaneous flame is assumed to consist of localized reactive sheets, which are transported by the flow and wrinkled by turbulent eddies. The flamelet approach is applicable when the characteristic turbulent scales are larger than a typical flame thickness. This condition is satisfied in many practical situations. The flamelet models are usually based on the flame surface density concept or apply probability density functions. One of the most attractive flamelet models is based on the balance equation for the flame surface density. This equation governs the transport of the mean reactive surface by the turbulent flow and includes physical mechanisms responsible for flame surface area production and destruction.

The approach used within this study is also based on considering the flame surface area. However, to speed up calculations, instead of solving the partial differential equation for the flame surface density, it implies tracing of the mean reactive surface and application of the laminar/turbulent flame velocity concepts.

2 FLAME TRACKING METHOD

The approach outlined below will be referred to as the subgrid model of laminar/turbulent combustion. First, explain the essence of the model on the example of laminar flame propagation. The flame surface shape and area can be found based on the Huygens principle: Each elementary portion of the flame surface displaces in time due to burning of the fresh mixture at local velocity $u_n$ (normal to the flame surface) and due to convective motion of the mixture at local velocity $u$. The local instantaneous velocity $u_n$ can be taken from the lookup tables.
including in general the effects of mixture dilution with combustion products, flame stretching, and flammability limits. The local instantaneous velocity $u$ can be calculated using a CFD code and high-order interpolation technique. In 2D flow approximation, the flame surface is represented by straight line segments, whereas in 3D calculations, the flame surface is represented by connected triangles.

The energy release rate in a computational cell, $\dot{Q}$, is composed of two terms: energy release due to frontal combustion, $\dot{Q}_f$, and energy release due to volumetric reactions, $\dot{Q}_v$. The first term $\dot{Q}_f$ can be calculated based on the estimated instantaneous flame surface area $S_n$ and the laminar flame propagation velocity $u_n$:

$$
\dot{Q}_f = \rho Q \sum_i S_{ni} u_{ni}
$$

where $\rho$ is the density of the reactive mixture, $Q$ is the combustion heat, and summation is made over all flame segments in the cell. The second term $\dot{Q}_v$ can be calculated using a Particle method (see Section 3).

In the turbulent flow field, a pulsating velocity vector distorts the “mean” reactive (flame) surface by wrinkling it. The local instantaneous flame wrinkling can be taken into account by proper increasing the normal flame velocity or, in other words, by introducing a concept of local turbulent flame velocity $u_t$. The local turbulent flame velocity is defined as

$$
u_t = \frac{u_n S}{S_t}
$$

where $S$ is the surface area of the wrinkled flame at a given segment and $S_t$ is the surface area of the equivalent “planar” flame.

The problem now is to find the way of calculating $u_t$. In the theory of turbulent combustion, there are many correlations between $u_t$ and $u_n$. One of classical correlations is Shchelkin formula [4]:

$$
u_t \approx u_n \sqrt{1 + \frac{u'^2}{u_n^2}}
$$

where $u'$ is the local turbulence intensity, related to the turbulent kinetic energy or to pulsating velocity correlations. Instead of Eq. (1), one can use other available correlations for the turbulent flame velocity.

One can apply the Huygens principle to model only the “mean” shape of the turbulent flame: each elementary portion of flame surface displaces in time due to burning of the fresh mixture at local velocity $u_t$ (normal to the flame surface) and due to convective motion of the mixture at local velocity $u$.

In the turbulent flow field, the mean energy release rate in a computational cell, $\bar{Q}$, is also composed of two terms: energy release due to frontal combustion, $\dot{Q}_f$, and energy release due to volumetric combustion, $\dot{Q}_v$. The first term
\( \dot{Q}_f \) can be calculated based on the estimated "mean" flame surface area and the turbulent flame propagation velocity using Eq. (1) (or other correlations). Equation (1) relates the turbulent flame velocity to laminar flame velocity (tabulated) and local turbulence intensity (provided by any model of turbulence). Based on such an equation, one can calculate the mean (frontal) energy release rate in the computational cell as the sum

\[
\dot{Q}_f = \rho Q \sum S_{ti} u_{ti}
\]

where index \( i \) relates to the \( i \)th flame surface segment in the cell. The second term \( \dot{Q}_v \) can be calculated using a Particle method (see Section 3).

Thus, the subgrid model of turbulent premixed combustion does not differ much from that of the laminar premixed combustion, except for using \( u_t \) instead of \( u_n \). Moreover, the formulae like Eq. (1) are asymptotically valid for the subgrid model of laminar combustion (when \( u' \to 0, u_t \sim u_n \)). It stands to reason that the turbulent combustion model will be also valid for the laminar combustion as a limiting case. This is one of model advantages. This feature will allow using the same model to calculate the initial laminar flame kernel growth from the spark ignition with continuous transition to turbulent combustion. The subgrid combustion model under consideration does not contain tuning parameters (some parameters can be introduced with the equations replacing Eq. (1)). This is the other important model advantage. The additional advantage of the model is that, when coupled with the Particle method, it will cover both possible modes of premixed combustion, namely, frontal and volumetric.

It is expected that the accuracy of the computational results will be mainly affected by the turbulence model used. The main problem in implementing such a combustion model into a CFD code is the development of an efficient algorithm for "mean" flame-shape tracing inside computational cells. This algorithm should meet the constraints on the flame-front continuity, connectivity, etc., and the constraints on the CPU time consumption.

### 3 PARTICLE METHOD

The Particle method allows continuous monitoring of preflame reactions. The preflame zone exhibits volumetric reactions of fuel oxidation, formation of intermediate products like alcohols, aldehydes, peroxides, etc. In general, the preflame reactions are inhomogeneous due to inhomogeneous distributions of temperature and species concentrations. The preflame reactions can result in the localized energy release. For example, low-temperature cool-flame oxidation of \( n \)-alkane fuels can result in the release of up to 10%–15% of the total reaction heat. Thus, in general, two-way coupling approach has to be applied for the preflame reactions; however, in some cases, one-way coupling is also possible.
The direct (and CPU time consuming) way to calculate the volumetric reaction rates is to solve the equations of chemical kinetics in the preflame zone in each computational cell with due regard to turbulence–chemistry interaction. To shorten the CPU time, one can introduce a certain number of trace (notional) Lagrangian particles which will move in the preflame zone according to the local velocity vector. In each particle, the preflame reactions will proceed at the rates determined by its instantaneous temperature and species concentrations. For determining the time and location of preflame autoignition, there will be a need in adopting a certain criterion. Such a criterion can be based on the fixed rate of temperature rise in the particles, e.g., 10⁶ or 10⁷ K/s.

In case of two-way coupling, the ignition delay is calculated in each particle based on its temperature and species concentrations and the mean (over all particles in cell) reaction rate directly affects the mean flow pattern. When an autoignition criterion is met in one or several particles, new (forced) ignition sites in the preflame zone can be automatically introduced. In general, these ignition sites give birth to new laminar/turbulent flame kernels or, if the preflame reactions are fast, they result in the induction (spontaneous) flames and volumetric combustion. The number of particles in the preflame zone can be less than the number of computational cells. For keeping the number of particles at a reasonable level, the consistent procedures of particle cloning and clustering should be developed. The preflame particles are traced until the entire geometry is traversed by the frontal or volumetric combustion.

In each $i\text{th}$ Lagrangian particle, the following set of equations is solved [14]:

- **Equation of motion:**
  \[
  \frac{dx^i_k}{dt} = u^i_k
  \]
  where $x^i_k$ is the coordinate ($k = 1, 2, \text{and } 3$); and $u^i_k$ is the velocity component;

- **Mass conservation equation:**
  \[
  \frac{d\left(\rho^i V^i\right)}{dt} = \nabla J^i_l + J^i_l
  \]  \hspace{1cm} (2)
  where $\rho^i_l$ is the partial density of the $l$th species; $V^i$ is the particle volume; $\nabla J^i_l$ is the diffusion flux of the $l$th species to/from the particle; and $J^i_l$ is the flux of the $l$th species due to chemical reaction;

- **Momentum conservation equation:**
  \[
  \rho^i \frac{du^i_k}{dt} = \frac{\partial P^i}{\partial x_k} - \nabla (Ip^i + \tau^i)
  \]  \hspace{1cm} (3)
where \( \rho^i \) is the mean particle density \( (\rho^i = \sum \rho^i_l) \); \( P^i \) is the mean pressure; \( p^i \) is the pulsating pressure; \( I \) is the unit tensor; and \( \tau^i \) is the molecular viscous stress;

- **Energy conservation equation:**

\[
\rho^i \frac{dh^i}{dt} = -\nabla q^i + h_{\text{hom}}^i + \frac{\partial P^i}{\partial t} - P \frac{\partial u_k^i}{\partial x_k} \tag{4}
\]

where \( h^i \) is the particle enthalpy; \( q^i \) is the heat flux to/from the particle; \( h_{\text{hom}}^i \) is the rate of heat release due to chemical reaction; \( \partial P^i / \partial t \) is the rate of particle heating due to adiabatic compression; and \( P \partial u_k^i / \partial x_k \) is the rate of particle heating due to shock compression. Note that the volumetric term \( Q_v \) mentioned above is calculated based on \( h_{\text{hom}}^i \).

Molecular diffusion term \( \nabla J^i_l \) in Eq. (2), molecular heat transfer term \( \nabla q^i \) in Eq. (4) and term \( \partial p^i / \partial x_k + \nabla \tau \) in Eq. (3) require modeling. These terms are modeled using classical models of interaction by exchange with the mean [15]:

- **Diffusion term:**

\[
\nabla J^i_l = -0.5C_1 \left( Y^i_l - \overline{Y}^i_l \right) \rho^i \omega
\]

where \( C_1 \) is the coefficient \( (C_1 \approx 2.0) \); \( Y^i_l \) is the concentration of the \( l \)-th species; \( \overline{Y}^i_l \) is the mean concentration of the \( l \)-th species in the location of the \( i \)-th particle; and \( \omega \) is the turbulent frequency.

- **Heat exchange term:**

\[
\nabla q^i = -0.5C_2 \left( h^i - \overline{h}^i \right) \rho^i \omega
\]

where \( C_2 \) is the coefficient \( (C_2 \approx 2.0) \); \( h^i \) is the enthalpy; and \( \overline{h}^i \) is the mean enthalpy in the location of the \( i \)-th particle.

- **Term \( \nabla (Ip^i + \tau^i) \):**

\[
(\rho^i)^{-1} \nabla (p^i I + \tau^i) = -\zeta \left( u_k^i - \overline{u}^i_k \right) + A(t)
\]

where \( \overline{u}^i_k \) is the mean velocity in the location of the \( i \)-th particle; \( \zeta \) is the coefficient \( (\zeta \approx 2.075 \omega) \); and \( A(t) \) is the stochastic function in the Langevin equation.

For effective implementation of the Particle method, the reaction rate term \( J^i_l \) in Eq. (2) and heat release term \( h_{\text{hom}}^i \) in Eq. (4) can be neglected in those preflame domains where the local temperature is less than a certain conditional value \( T_c \). This assumption allows omitting routine chemical kinetic calculations in the
major part of the preflame zone with $T < T_c$. Thus, each computational cell contains a certain number $N$ of particles with $N$ chosen to support a proper statistical accuracy. The preflame domain is then represented by stochastically moving “cold” (with $T < T_c$) and “hot” (with $T \geq T_c$) notional Lagrangian particles (Fig. 1). In long tubes with one open end (like a PDE tube), most of particles are “cold” and routine kinetic calculations for them are not required. “Hot” particles are concentrated in the region between a flame-induced shock wave and the flame itself.

### Table 1 Laminar flame velocities for the stoichiometric propane–air mixture (cm/s)

<table>
<thead>
<tr>
<th>Pressure, MPa</th>
<th>Temperature, K</th>
<th>300</th>
<th>450</th>
<th>600</th>
<th>750</th>
<th>900</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>39</td>
<td>78</td>
<td>143</td>
<td>247</td>
<td>451</td>
<td></td>
</tr>
<tr>
<td>0.3</td>
<td>28</td>
<td>55</td>
<td>102</td>
<td>178</td>
<td>306</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>19</td>
<td>35</td>
<td>64</td>
<td>112</td>
<td>191</td>
<td></td>
</tr>
<tr>
<td>4.0</td>
<td>8.9</td>
<td>19</td>
<td>36</td>
<td>62</td>
<td>105</td>
<td></td>
</tr>
<tr>
<td>10.0</td>
<td>6.0</td>
<td>13</td>
<td>24</td>
<td>41</td>
<td>69</td>
<td></td>
</tr>
</tbody>
</table>

4 KINETIC DATABASE

The coupled FTP algorithm is supplemented with the database of tabulated laminar flame velocities for the stoichiometric propane–air mixture in the wide range of initial temperature and pressure (Table 1) as well as the reaction kinetics of preflame fuel oxidation [14] (Tables 2 and 3).

### Table 2 Reaction mechanism of preflame propane oxidation

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$H$, kcal/mol</th>
<th>Forward</th>
<th>Reverse</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reaction 1:</td>
<td>$C_3H_8 + 3.5O_2 \rightarrow 3CO + 4H_2O$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reaction 2:</td>
<td>$CO + H_2O \leftrightarrow CO_2 + H_2$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reaction 3:</td>
<td>$H_2 + H_2 + O_2 \rightarrow H_2O + H_2O$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reaction 4:</td>
<td>$CO + CO + O_2 \rightarrow CO_2 + CO_2$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$H$, kcal/mol</th>
<th>$A$, mol, l, s</th>
<th>$a$</th>
<th>$E$, kcal/mol</th>
<th>$A$, mol, l, s</th>
<th>$a$</th>
<th>$E$, kcal/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>290.0</td>
<td>$A_1$</td>
<td>0.0</td>
<td>$E_1$</td>
<td>3.1 $\cdot 10^{13}/P$</td>
<td>0.0</td>
<td>49.1</td>
</tr>
<tr>
<td>2</td>
<td>10.0</td>
<td>$1.0 \cdot 10^{12}/P$</td>
<td>0.0</td>
<td>41.5</td>
<td>$1.0 \cdot 10^{12}/P$</td>
<td>0.0</td>
<td>21.0</td>
</tr>
<tr>
<td>3</td>
<td>114.0</td>
<td>$7.0 \cdot 10^{13}/P^{0.5}$</td>
<td>0.0</td>
<td>21.0</td>
<td>$8.5 \cdot 10^{12}/P^{1.5}$</td>
<td>0.0</td>
<td>21.0</td>
</tr>
</tbody>
</table>

**Remarks:**
1. Reaction rate constant is defined as: $k = AT^a \exp(E/(RT))$.
2. Reaction 1 is considered as bimolecular.
3. Pressure $P$ is taken in atmospheres.
Note that the reaction mechanism of Tables 2 and 3 describes a two-stage low-temperature autoignition of propane at \( T < 775 \text{ K} \) [16]. In this case, the temperature history of the mixture in an adiabatic reactor exhibits two stages: “cool flame” with the induction period \( \tau_1 \) and subsequent “hot explosion” with the induction period \( \tau_2 \). The overall induction period is \( \tau = \tau_1 + \tau_2 \). To obtain such a behavior of the temperature curve based on Tables 2 and 3, one has to use two different sets of kinetic parameters for the rate limiting reaction 1: one at \( T < 775 \text{ K} \) (see Table 3, column 2) and another at \( T > 775 \text{ K} \) (see Table 3, column 3).

### Table 3 Kinetic parameters of rate limiting reaction 1

<table>
<thead>
<tr>
<th>( p, \text{ atm} )</th>
<th>( A_1, \text{l/(mol·s)} )</th>
<th>( A_1, \text{l/(mol·s)}^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.96 ( \cdot ) 10(^{12} ) ( P )</td>
<td>1.73 ( \cdot ) 10(^{12} / P^{0.2264} )</td>
</tr>
<tr>
<td>20</td>
<td>1.96 ( \cdot ) 10(^{12} ) ( P )</td>
<td>8.77 ( \cdot ) 10(^{11} / P^{0.2264} )</td>
</tr>
<tr>
<td>40</td>
<td>1.96 ( \cdot ) 10(^{12} ) ( P )</td>
<td>7.50 ( \cdot ) 10(^{11} / P^{0.2264} )</td>
</tr>
<tr>
<td>80</td>
<td>1.96 ( \cdot ) 10(^{12} ) ( P )</td>
<td>6.41 ( \cdot ) 10(^{11} / P^{0.2264} )</td>
</tr>
<tr>
<td>120</td>
<td>1.96 ( \cdot ) 10(^{11} ) ( P )</td>
<td>5.85 ( \cdot ) 10(^{11} / P^{0.2264} )</td>
</tr>
</tbody>
</table>

**Remarks:**

1) \( T < 775 \text{ K} \) and \( E_1 = 40 \text{ kcal/mol} \).
2) \( T > 775 \text{ K} \) and \( E_1 = 45 \text{ kcal/mol} \).

### 5 RESULTS OF CALCULATIONS

#### 5.1 Validation

The coupled FTP method has been developed and implemented into the standard CFD code (here, AVL FIRE). The results of integrated code validation for flame propagation in enclosures including the effects of two-stage preflame autoignition are presented elsewhere [17]. As an example of FTP method performance for accelerating flames in tubes with one open end, consider the results of three test cases with flame acceleration in the straight cylindrical tube of internal diameter \( D = 152 \text{ mm} \) and length \( L = 3.1 \text{ m} \) with regular obstacles in the form of orifice plates with blockage ratio (BR) 0.43, 0.6, and 0.75 filled with the stoichiometric propane–air mixture at normal initial conditions as used in experiments [18].

The BR of orifice plates was defined as \( \text{BR} = 1 - (d/D)^2 \) where \( d \) is the orifice diameter. In the experiments, the mixture was initially quiescent and spark ignition took place at the closed end of the tube.

The geometries of the tubes were represented by axisymmetrical geometries. The tube walls were assumed isothermal (\( T_w = 293 \text{ K} \)). At the open end, a constant-pressure \( (p_0 = 0.1 \text{ MPa}) \) boundary condition was applied. The use of nonreflecting boundary conditions [19] at the walls of a buffer volume of a larger cross section attached to the open end of the tube did not affect significantly the results of calculations leading, however, to increasing CPU time. The stoichiometric propane–air mixture was assumed initially quiescent at \( T_0 = 293 \text{ K} \) and \( p_0 = 0.1 \text{ MPa} \). The initial flame kernel was taken as a circle 1 mm in radius with the center located at 1 cm from the closed endwall at the symmetry axis. The turbulent flame velocity was modeled by the Shchelkin formula (Eq. (1)). The lami-
Figure 2 Predicted (curves) and measured (symbols [18]) visible flame velocities vs. distance in tubes of $D = 152$ mm with regular orifice plates (BR = 0.43 (1), 0.6 (2), and 0.75 (3), pitch $S = D$). Stoichiometric propane-air mixture at $T_0 = 293$ K and $p_0 = 1$ atm.

Figure 2 compares predicted visible flame velocities (curves) with experimental data [18] (symbols) depending on the distance traveled by the flame for the three different values of BR. In all cases, the distance between neighboring orifice plates (pitch $S$) was equal to tube diameter, $S = D$.

In general, satisfactory agreement between predicted and measured values of flame velocity is worth mentioning. Very good agreement is attained at the initial phase of flame acceleration where its velocity is less than 300–400 m/s. The flame accelerates to about 800–900 m/s, i.e., to the velocity close to the sound speed in the combustion products (about 890 m/s). Initially, the flame accelerates faster in the tube with orifice plates of larger BR. This is probably caused by a higher level of turbulence generated by such obstacles. However, further flame acceleration results in growing momentum losses and the efficiency of orifice plates with high BR in terms of flame acceleration decreases.

5.2 Calculations of Deflagration-to-Detonation Transition

Figure 3 shows the schematic of a planar PDE channel (channel height $H = 52$ nm, $L = 3$ m) containing four segments: (i) flame acceleration segment 1.28 m long with one closed end and regular obstacles in the form of orifice plates with BR = 0.25 and pitch $S = 20$ mm; (ii) first smooth-walled segment 0.22 m
(iii) shock-wave focusing element 0.5 m long in the form of the converging-diverging (CD) nozzle of a special shape; and (iv) second smooth-walled segment 1 m long with an end open to the atmosphere. The PDE configuration containing “flame accelerator” and “shock focusing element” has been first suggested in [20] for implementing a fast DDT concept [21, 22]. It implies that a shock wave generated by the accelerating flame can be transformed into a detonation wave while passing through the shock focusing element (tube coil, U-bend, CD nozzle, etc.). The converging part of the CD nozzle ensures shock-to-detonation transition in the core flow behind the nozzle throat, whereas the conical diverging part ensures detonation survival and transitioning to the smooth-walled channel of height $H$.

The first (intermediate) smooth-walled segment is used for ensuring a plug flow of shock-compressed unreacted mixture of duration sufficient for shock-to-detonation transition in the nozzle. The nozzle geometry was the same as that successfully tested experimentally in [22] with the stoichiometric propane-air mixture.

The reactive mixture in the PDE channel was assumed initially quiescent at $T_0 = 293$ K and $p_0 = 0.1$ MPa and filling the entire geometry. The walls of the channel were assumed isothermal ($T_w = 293$ K). At the open end, a large-volume buffer section with initial pressure $p_0 = 0.1$ MPa was attached to the PDE channel.

The boundary conditions and ignition were modeled in the same way as described above. In planar 2D calculations, only an upper half of the PDE channel was considered with symmetry boundary conditions along three longitudinal symmetry planes. For tracing possible autoignition events, the preflame zone was filled with notional particles. The number of particles in each computational cell was controlled to be no less than 5 and no more than 20 with the mean value of 10. The autoignition of a particle was assumed to occur when the rate of temperature rise in this particle exceeded $10^6$ K/s. The two-way coupling procedure between the particles and the mean flow was used. The autoignition of at least one particle in a cell was treated as the autoignition of the mixture all throughout the cell volume.
DEFLAGRATIVE AND DETONATIVE COMBUSTION

Figure 4 shows the predicted time histories of visible flame and lead shock wave velocities. In the flame acceleration segment, both the flame and lead shock velocities increase to about 980 m/s.

Upon entering the first smooth-walled segment, the flame starts decelerating whereas the shock wave continues propagating with nearly constant velocity and attains the velocity of $\sim 1100$ m/s at the nozzle inlet. The diagram of Fig. 4 indicates shock-to-detonation transition in the nozzle. The detonation wave is initiated via the overdriven detonation mode. The maximum degree of overdrive is 1.26. When the detonation wave enters the second smooth-walled segment, the degree of its overdrive is 1.03. The overdriven detonation further decays to the self-sustained CJ mode in the second smooth-walled segment with the constant velocity close to 1900 m/s. This velocity corresponds to the thermodynamically equilibrium value calculated based on the composition of reaction products provided by Table 2 ($\text{CO}_2, \text{H}_2\text{O}, \text{CO}, \text{H}_2, \text{C}_3\text{H}_8, \text{and O}_2$). Note that this value is about 5% higher than the thermodynamic detonation velocity $D_{\text{CJ}} \approx 1804$ m/s calculated based on the extended composition of reaction products [23, 24].

Figure 5 shows the snapshots of temperature and pressure fields at several time instants ($t = 20, 21$, and $21.5$ ms after ignition) during flame propagation in the flame accelerating segment. In the course of flame propagation along the channel, its overall shape exhibits various transformations, including a tulip-like shape (not shown in Fig. 5) in qualitative accordance with experimental observations. The local instantaneous flame wrinkling increases with time. At 20 ms, the bell-shaped flame is elongated with the characteristic length of about $4H$ between the lead central point and the attachment point at the channel wall. The elongation of the flame rapidly decreases with time: at $t = 21$ ms, it drops to $2H$ and at $t = 21.5$ ms, to $1.5H$. At $t = 21.5$ ms, a shock wave with abrupt temperature and pressure rise is clearly seen ahead of the flame. Also seen are intense bow shocks attached to the obstacles which are the indication of super-
FUNDAMENTALS OF DEFLAGRATION-TO-DETONATION TRANSITION

Figure 5 Predicted temperature (top) and pressure (bottom) fields at $t = 20$ (a), $21$ (b), and $21.5$ ms (c) after ignition

sonic shock-compressed flow ahead of the flame. Noteworthy is a short distance between the lead flame point and the flame-generated shock wave (about $1.2H$). As is seen, the FTP method avoids numerical diffusion of scalar variables through the flame front: the infinitely thin flame is always concentrated inside one computational cell, thus separating unburned mixture from combustion products in this cell.

Figure 6 is the continuation of the snapshot sequence in Fig. 5 for $t = 21.95$, $21.975$, $22.0$, and $22.025$ ms after ignition. These snapshots correspond to the stage of the process after the shock wave–flame complex leaves the flame accelerating segment. At $t = 21.95$ ms, the shock wave–flame complex propagates in the first smooth-walled segment of the PDE channel. Due to low turbulence intensity in this section, the flame lags behind the shock wave thus the distance between them increases to about $2H$. At $t = 21.975$ ms, the shock wave reflects from the converging nozzle wall creating several clusters of exothermic centers clearly seen in both pressure and temperature snapshots. The hot spots are located at the converging nozzle surface. At $t = 22.0$ ms, the reflection-induced preflame autoignition (“explosion in the explosion” [5]) gives rise to an extended region with extremely fast volumetric combustion. This explosion generates an
Figure 6 Snapshots of temperature and pressure fields prior, at and after shock-to-detonation transition (the transversal size of the tube is purposely increased to clarify the details): (a) $t = 21.95$ ms; (b) 21.975; (c) 22.0; and (d) $t = 22.025$ ms after ignition.
overdriven detonation in the rear and frontal parts of the region. The wave propagating towards the flame is usually referred to as a retonation wave: when passing through the flame, it degenerates to a nonreactive shock wave propagating in the combustion products. The wave propagating outwards from the flame is referred to as a detonation wave. Contrary to the relatively slow initial stage of flame acceleration, the evolution of the DDT process after preflame autoignition is very fast and occurs within about 50 \( \mu \text{s} \).

In the presence of preflame autoignition, two modes of combustion become possible simultaneously, namely the frontal and volumetric. Remind that the frontal mode is calculated using the Flame Tracking method whereas the volumetric mode is calculated using the Particle method. Formally, for adequate simulation of the DDT process, one has to take into account the transition of the volumetric mode to the frontal one, in particular, in relatively cold near-wall

\[\text{Figure 7} \quad \text{Predicted spatial pressure distributions in the PDE channel at different time (in ms) after ignition. Different pressure scales are used for } t < 21.9 \text{ ms (a) and } t > 21.9 \text{ ms (b)}\]
Figure 8 Predicted temperature (top) and pressure (bottom) fields at different time after ignition (snapshots correspond to time instants shown in Fig. 7 except for $t = 20$ ms). The transversal size of the tube is purposefully increased to clarify the details. (Refer color plate, p. VI.)
Figure 8  (Continued) Predicted temperature (top) and pressure (bottom) fields at different time after ignition (snapshots correspond to time instants shown in Fig. 7 except for $t = 20$ ms). The transversal size of the tube is purposefully increased to clarify the details. (Refer color plate, p. VII.)
DEFLAGRATIVE AND DETONATIVE COMBUSTION

regions. At this stage of code development, this transition is not taken into account. Despite this fact does not affect much the DDT run-up distance and time (the volumetric mode spreads very fast predominantly in the longitudinal direction), it can affect the completeness of combustion, and therefore, the detonation velocity and other parameters (pressure, etc.).

Figure 7 shows the predicted spatial pressure distributions in the PDE channel at different time after ignition. Pressure oscillations are caused by bow shocks and rarefaction waves generated by regular obstacles. The localized “explosion in the explosion” occurring at about 22 ms results in pressure rise up to 150 atm. Figure 8 shows the snapshots of temperature and pressure corresponding to all time instants presented in Fig. 7.

5.3 Thrust Performance

Finally, the thrust performance of the PDE under study is analyzed.

The solid curve in Fig. 9 shows the time history of the specific (per unit area) thrust defined as

\[
\mathcal{P}(t) = \frac{1}{F_e} \int_{F_e} \left[ \rho_e(t,y)U_e^2(t,y) + p_e(t,y) - p_0 \right] \, dF
\]

where \( F \) is the cross-section area of the PDE channel; \( \rho, U, \) and \( p \) are the gas density, velocity, and pressure, respectively; and index \( e \) relates to the PDE channel outlet. For the sake of convenience and due to different scales of the variable, Fig. 9a shows the specific thrust history for the early stage of the

\[\begin{array}{c}
\text{Figure 9} \quad \text{Time histories of the specific (per unit area) thrust calculated based on the exhaust flow parameters at the PDE channel exit: 1 — DDT in the PDE channel of Fig. 3; 2 — direct detonation initiation in a straight smooth-walled channel of Fig. 11; 3 — direct detonation initiation in the PDE channel of Fig. 3 for } t < 12 \text{ ms (a) and } 9 < t < 50 \text{ ms (b).}
\end{array}\]
exhaust process \((t < 12 \text{ ms})\) and Fig. 9b for its later stage \((9 < t < 50 \text{ ms})\) with some overlapping.

Define the impulse per unit area as

\[
I_{\text{DDT}} = \int_0^{t_{\text{ev}}} P(t) \, dt. \tag{6}
\]

Here, the upper index DDT is used to identify the impulse at DDT; \(t_{\text{ev}}\) is the PDE channel evacuation time (the time taken for \(P(t)\) to attain the zero value). The specific fuel-based impulse is then defined as

\[
I_{\text{DDT}}^{\text{sp}} = F_e \frac{I_{\text{DDT}}}{m_f g} \tag{7}
\]

where \(m_f\) is the fuel mass in the PDE channel and \(g\) is the acceleration of gravity. The integral of Eq. (6), i.e., the area under the solid curve in Fig. 9, is approximately \(I_{\text{DDT}} \approx 4880 \text{ Pa} \cdot \text{s}\). The estimated calculation error of \(I_{\text{DDT}}\) is 2\%, i.e., \(I_{\text{DDT}} \approx 4880 \pm 100 \text{ Pa} \cdot \text{s}\). Taking into account that \(F_e = 0.026 \text{ m}^2/\text{m}, m_f \approx 0.0052 \text{ kg}/\text{m},\) and \(g = 9.8 \text{ m}/\text{s}^2\), one comes to the following value of the specific impulse \(I_{\text{DDT}}^{\text{sp}}\):

\[
I_{\text{DDT}}^{\text{sp}} = F_e \frac{I_{\text{DDT}}}{m_f g} \approx 0.026 \frac{4880}{0.0052 \cdot 9.8} \approx 2480 \pm 50 \text{ [s]} \tag{8}
\]

Note that this value has been obtained based on Eqs. (5) and (6), i.e., based on momentum integration at the PDE outlet. Thus, the value of 2480 ± 50 s should be treated as the net specific impulse at PDE full fill conditions.

Obviously, this value of the specific impulse should be identical to the value obtained by direct integration of the pressure over the projection of all PDE channel surfaces on the plane normal to \(y\)-axis (see Fig. 3). This fact can be used for estimating the values of momentum and energy losses in the PDE channel with regular obstacles and a CD nozzle. Such an estimate can be obtained by comparing the specific impulse \(I_{\text{sp}}^{\text{DDT}}\) of Eq. (8) with that calculated based on the pressure history at the closed end (thrust wall). The difference can be readily attributed to the losses.

Figure 10 shows the calculated time history of pressure \(P_T\) at the thrust wall. Defining the force acting at the unit area of the thrust wall \(P_T\) and impulse per unit area \(I_T^{\text{DDT}}\) as

\[
P_T(t) = \frac{1}{F_t} \int F_T(t) - p_0 \, dF_T \tag{9}
\]

and

\[
I_T^{\text{DDT}} = \int_0^{t_{\text{ev}}} P_T(t) \, dt \tag{10}
\]
DEFLAGRATIVE AND DETONATIVE COMBUSTION

(where index $T$ relates to the thrust wall), one obtains

$$I_{sp,T}^{DDT} = F_T \frac{I_{sp}^{DDT}}{m_f g} \approx 0.026 \frac{5060}{0.0052 \cdot 9.8} \approx 2580 \text{ [s]}.$$  \hspace{1cm} (11)

Since the value of $I_{sp,T}^{DDT}$ is calculated more precisely than $I_{sp}^{DDT}$, the difference between these values can be estimated as $\Delta I_{sp}^{DDT} = I_{sp}^{DDT} - I_{sp,T}^{DDT} \approx -100 \pm 50 \text{ s}$. This difference should be obviously attributed to momentum and energy losses of the flow in the PDE channel caused by obstacles, CD nozzle, and cold walls.

The relative contribution of the losses is unexpectedly very small: $\Delta I_{sp}^{DDT}/I_{sp}^{DDT} \approx 0.02-0.06$. By other words, the specific impulse of the PDE under study can be estimated based on the thrust wall pressure $p_T$.

For better understanding the results obtained, some additional calculations have been made. Thus, in addition to the PDE configuration of Fig. 3, the 2D configuration with a straight smooth-walled PDE channel of the same height ($H = 52 \text{ mm}$) and length ($L = 3 \text{ m}$) but with direct detonation initiation was also considered (Fig. 11). The detonation was initiated at the closed end of the PDE channel by making a provision for the high-pressure (40 atm) initiation section with the length $l = H$ filled with hot combustion products of the stoichiometric propane–air mixture at initial temperature 3300 K. To facilitate detonation initiation, the initial velocity of the products was taken equal to 2000 m/s. Clearly, for the PDE channel of Fig. 11, the specific impulse can be estimated using either Eqs. (5)–(7) or Eqs. (9)–(11) with a good accuracy (skin friction and heat losses can be neglected).

The dashed curve 2 in Fig. 9 shows the specific thrust history at the outlet of the PDE channel for this case. The area under the dashed curve 2 in Fig. 9

**Figure 10** Predicted absolute pressure history at the head end of the PDE tube (PDE thrust wall)

**Figure 11** Schematic of a straight smooth-walled PDE channel with a section for direct detonation initiation. Dimensions are in millimeters
is approximately equal to $I_{2D}^{2D} \approx 5040 \pm 100 \text{ Pa·s}$ (from now on, upper index 2D relates to the 2D calculation for the straight smooth-walled PDE channel), which is somewhat larger than for that under the solid curve ($I_{DDT}^{2D} \approx 4880 \pm 100 \text{ Pa·s}$). Taking into account that the fuel mass in the PDE channel of Fig. 11 is somewhat larger ($m_f^{2D} \approx 0.00547 \text{ kg/m}$) than in the PDE configuration of Fig. 3, one comes to the following value of the specific impulse $I_{sp}^{2D}$:

$$I_{sp}^{2D} = F_e \frac{I_{2D}^{2D}}{m_f^{2D} g} \approx 0.026 \frac{5040}{0.00547 \cdot 9.8} = 2440 \pm 50 \text{ s}$$

or

$$I_{sp}^{DDT} \approx I_{sp}^{2D},$$

i.e., the DDT process in the PDE channel with obstacles and CD nozzle provides the same specific impulse as a detonation in a straight channel of the same length and nearly the same fuel mass. One has to take into account that contrary to $I_{sp}^{DDT}$, the value of $I_{sp}^{2D}$ is affected by the contribution of detonation initiator [25]. According to [25], depending on the tube length and initiator energy, the initiator contribution to the impulse can be as large as 17% to 27%.

It is instructive to compare the present results of numerical simulation in the straight smooth-walled PDE channel with the results available in the literature. According to one-dimensional (1D) analysis [24, 25], the impulse per unit area $I_{1D}$ is equal to

$$I_{1D} \approx K (p_{TZ} - p_0) t_{CJ}$$

where upper index 1D relates to 1D analysis, $t_{CJ} = L / D_{CJ}$ is the residence time of the detonation in the PDE channel, $p_{TZ}$ is the Taylor–Zel’dovich “detonation kernel” pressure, and $K$ is the coefficient which is different in various studies due to details of direct detonation initiation, channel geometry, etc.: $K = 4.65$ in [25], 4.85 in [26], and 5.15 in [24]. The value of $p_{TZ}$ can be calculated as [24]:

$$p_{TZ} = p_{CJ} \left( \frac{\gamma + 1}{2\gamma} \right)^{2\gamma/(\gamma - 1)}$$

where $p_{CJ}$ is the CJ pressure and $\gamma$ is the ratio of specific heats in the detonation products. For the stoichiometric propane–air mixture at normal initial conditions, $p_{CJ} = 1.827 \text{ MPa}$ and $\gamma \approx 1.166$; therefore, $p_{TZ} \approx 0.65 \text{ MPa}$. The “ideal” residence time in the example under consideration is $t_{CJ} \approx 3/1804 \approx 1.66 \text{ ms}$. Substituting these values in Eq. (12) gives

$$I_{1D} \approx 4250 - 4700 \ [\text{Pa·s}].$$

The corresponding value of the specific impulse is

$$I_{sp}^{1D} \approx 2010 - 2230 \ [\text{s}].$$
These values are less than those obtained in the present 2D calculations ($I_{2D} \approx 5040 \pm 100 \, \text{Pa} \cdot \text{s}$ and $I_{2D}^{sp} \approx 2390 \pm 50 \, \text{Pa} \cdot \text{s}$). The excess impulse in the present calculations (about 13% in average) can be explained, e.g., by the contribution of the detonation initiator.

Another additional calculation was made for the PDE configuration of Fig. 3, but instead of DDT, direct detonation initiation was applied. The initiation technique was the same as in Fig. 11. The specific thrust history at the PDE channel outlet for this case is shown by the dotted curve in Fig. 9. Since the area under the dotted curve in Fig. 9 is approximately equal to $I_D \approx 4180 \pm 80 \, \text{Pa} \cdot \text{s}$ and $m_f^D = m_f \approx 0.0052 \, \text{kg/m}$ (upper index $D$ relates to the values in a PDE channel of Fig. 3 with direct detonation initiation), the calculated value of $I_{sp}^D$ is equal to

$$I_{sp}^D = F_e \frac{I_D}{m_f g} \approx 0.026 \frac{4180}{0.0052 \cdot 9.8} = 2130 \pm 40 \, [\text{s}]$$

which is considerably (by 12%) less than $I_{sp}^{DDT} \approx 2480 \pm 50 \, \text{s}$. This result means unambiguously that overall momentum and energy losses at direct detonation initiation are higher than at DDT, in particular, in the obstructed segment of the PDE channel. Since the momentum losses are proportional to $\rho U^2$ [27], propagation of detonation in this segment of the channel is accompanied with higher momentum losses than in the course of flame acceleration. As for the intensity of heat losses, it is known to be higher for flows with higher Reynolds number, i.e., in a detonation wave. It is noteworthy that detonation requires a much shorter time for channel evacuation than a DDT.

6 CONCLUDING REMARKS

A coupled FTP method combined with the lookup tables of laminar flame velocities and fuel oxidation has been developed and implemented into the CFD code. The method is parameter free and very efficient in terms of CPU requirements. It avoids numerical diffusion of scalar variables through the flame front and provides spatial and temporal resolution of preflame autoignition sites. The algorithm has been tested for several 2D configurations with flame acceleration in smooth-walled channels of different length and with DDT in a channel with regular obstacles and demonstrated good solution convergence and stability. The numerical simulation of DDT in the stoichiometric propane–air mixture filling a PDE channel with regular obstacles and CD nozzle made it possible to estimate the fuel-based specific impulse on the level of 2480 ± 50 s which is very close to the value obtained for direct detonation initiation in a straight smooth-walled PDE channel of the same length. This result indicates that detonation initiation via DDT is a promising way in terms of propulsion efficiency. However, one has to keep in mind that the realistic PDE operation process additionally requires a
finite time for filling the PDE channel with the reactive mixture before ignition and purging the channel with air after combustion products exhaust into the atmosphere. Therefore, the cycle-averaged value of the specific impulse can be somewhat different from the predicted value.

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REFERENCES


