Numerical Study of Rotating Detonation Onset in Engines

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1 Abstracts

3D numerical modeling of a rotating detonation engine (RDE) combustion chamber is performed based on the original code. The RDE is a new type of engines capable to create higher thrust than the traditional ones based on the combustible mixture deflagration process. The dynamical process of combustion in the RDE is more than 100 times faster than in case of usual slow combustion. This type of an engine has more efficient thermal dynamics.

The combustion chamber under consideration is a co-axial hollow cylinder. The fuel is injected from one side, either premixed with the oxidizer, or from separate injectors. It is ignited in the chamber near the injectors, and this invokes the self-sustaining detonation wave which is then rotates consuming the combustible mixture. The burnt gases are expanded in the central part of the chamber where the internal hollow body changes from cylinder to cone and then vanishes. After the expansion, they leave the chamber from the side opposite to the injectors. The primary ignition is modeled by an energy source strong enough to produce an instant detonation wave.

The calculations are based on the Navier – Stokes system of equations along with the equations for turbulence modeling and the chemical kinetics. The computational domain used a regular mesh of uniform cubic elements. The time-critical program parts were parallelized using the OpenMP technique. Our calculations were made at APK-5 with a peak performance of 5.5 Tera Flops.

2 Introduction

A study and development of detonation engines is of a great interest nowadays. The efficiency of modern engines based on the traditional design is now close to its technological limit. The engines performance may be increased only with the use of new technical solutions. Within the last 20 years, there has been a

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considerable amount of research on developing engines utilizing detonation waves for air-breathing propulsion, to the point where propulsion engines are being developed and tested. Contrary to other types of detonation engines, the rotating detonation engine (RDE) uses a different approach toward ensuring the efficiency of the detonation cycle [1,2].

The RDE utilizes the high-efficiency detonation mode to organize the combustion process in the chamber. Fuel and oxidizer are injected into the combustion chamber at one end, and one or more detonation waves propagate circumferentially at the head of combustion chamber consuming the fresh mixture. The products leave the combustion chamber at the other end with high axial speed to produce the thrust Fig 1. Compared to pulse detonation engines (PDE's), the RDE can operate continuously once initiated, and the operating frequency is much higher than that of the PDE. Additionally, the RDE has a compact configuration, and can operate under a wide-range Mach-number condition. Therefore, the RDE has received a lot of attention in the propulsion research field. [3-10]

3 An Example of a Simple Equation

The mathematical model contains the governing equations (differential and algebraic), boundary and initial conditions. The details of the numerical realization together with the computational mesh design and the placement of variables on the mesh, is a subject of the numerical model.
The balance equations:

$$\frac{\partial \rho_k}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho_k u_j\right) - \frac{\partial J_{k,j}}{\partial x_j} = \dot{\omega}_k \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{i,j}}{\partial x_j} = 0 \tag{2}$$

$$\frac{\partial E_T}{\partial t} + \frac{\partial}{\partial x_j}\left(\left(E_T + p\right)u_j\right) - \frac{\partial}{\partial x_j}\left(J_{T,j} + u_i \tau_{i,j}\right) = \dot{Q} \tag{3}$$

Additional algebraic relations:

$$\rho = \sum_{k=1}^{N_C} \rho_k, Y_k = \frac{\rho_k}{\rho}, X_k = \frac{\rho_k}{W_k} \tag{4}$$

$$p = \tilde{p} + \frac{2}{3}\rho K, \tilde{p} = R_G T \sum_{k=1}^{N_C} X_k \tag{5}$$

The total energy of a volume unit is the following sum:

$$E_T = E + \rho\frac{u^2}{2} + \rho K, u^2 = u_j u_j \tag{6}$$

The total energy is therefore the sum of internal (thermal and chemical) energy, kinetic, and turbulent energy. The internal energy of a volume unit is modeled as follows:

$$E = \sum_{k=1}^{N_C} X_k E_k(T) = R_G T \sum_{k=1}^{N_C} X_k \cdot \left(\hat{H}_k(T) - 1 \right) \tag{7}$$

Here, EK is an internal energy of a species mole. Those functions: dimensionless enthalpy and internal energy are the basis of the species thermodynamic description; for many species, they are either tabulated, or approximated with polynomials. In the current research, they are taken from [11]

Chemical kinetics: In the current research, the chemical sources depend on temperature T and the set of molar densities $X=\{X_k\}$; the sum of those sources is zero due to the law of mass conservation in chemical reactions:

$$\dot{\omega}_k = W_k \hat{\omega}_k(T, \mathbf{X}), \sum_{k=1}^{N_C} \dot{\omega}_k = 0 \tag{8}$$

Some more strict laws for chemical interactions exist, e.g. the conservation of mass for each element. Those laws are considered in the chemical mechanism, and some-times can reduce the computations and increase the precisity. A general form for the chemical sources is usually complex, and it consists of many nonlinear terms; a typical expression is as follows:

$$\hat{\omega}_k = \sum_r \nu_{r,k} \omega_r, \omega_r = M_r(\mathbf{X}) \left[k_{F,r}(M_r, T) \prod_j X_j^{\alpha_{r,j}} - k_{R,r}(M_r, T) \prod_j X_j^{\beta_{r,j}} \right] \tag{9}$$

In case of elementary reactions, the degrees for species in the expression (9) are the same with the input and output stoichiometric coefficients. The reverse reaction speed coefficients were calculated to provide the dynamical reach of chemical equilibrium in the case of zero fluxes and constant density and internal energy:

$$k_{B,r} = k_{F,r} \exp\left(\sum_{k=1}^{N_C} \nu_{r,k} \left(\hat{H}_k(T) - \hat{S}_k(T) - 1 \right) \right) \left(\frac{R_G T}{p_{ref}} \right)^{\sum_{k=1}^{N_C} \nu_{r,k}} \tag{10}$$

For each direct reaction, its coefficient is modeled with an Arrhenius formula.

Turbulence model and transport: The current research uses the Wilcox k-ω model:

$$\frac{\partial \rho K}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho K u_j \right) - \frac{\partial}{\partial x_j}\left(\left(\mu + \sigma^* \mu_T \right) \frac{\partial K}{\partial x_j} \right) = \tau_{i,j}^T \frac{\partial u_i}{\partial x_j} - \beta^* \rho K \omega \tag{11}$$

$$\frac{\partial \rho \omega}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho \omega u_j \right) - \frac{\partial}{\partial x_j}\left(\left(\mu + \sigma \mu_T \right) \frac{\partial \omega}{\partial x_j} \right) = \alpha \frac{\omega}{K} \tau_{i,j}^T \frac{\partial u_i}{\partial x_j} - \beta \rho \omega^2 \tag{12}$$

$$\mu_T = \rho \frac{K}{\omega} \tag{13}$$

$\boldsymbol{\alpha}$=5/9, $\boldsymbol{\sigma}=\boldsymbol{\sigma}^*$=1/2, $\boldsymbol{\beta}$=3/40, $\boldsymbol{\beta}^*$=9/100 are constant parameters of the Wilcox model.
To calculate the fluxes of mass and energy $\boldsymbol{J_{k,j}}$ and $\boldsymbol{J_{T,j}}$, and the stresses tensor deviator $\boldsymbol{\tau_{i,j}}$, we used a model taking into account the turbulent transport calculated by means of the Wilcox model. In most cases, the turbulent transport supersedes the molecular, and the last is made using simplified technique: constant Prandtl **Pr** and Schmidt **Sc** numbers hypothesis:

$$J_{k,j} = \left(\frac{\mu}{\mathrm{Sc}} + \frac{\mu_T}{\mathrm{Sc}_T} \right) \frac{\partial Y_k}{\partial x_j} \tag{14}$$

$$J_{T,j} = \left(\frac{\mu}{\mathrm{Pr}} + \frac{\mu_T}{\mathrm{Pr}_T} \right) \frac{\partial h}{\partial x_j} + \left(\mu + \mu_T \right) \frac{\partial K}{\partial x_j} \tag{15}$$

Here, ScT, PrT are constant turbulent Schmidt and Prandtl numbers, h=H/ρ is the enthalpy per mass unit, δi,j is the Kronecker symbol.

4 The test problem

A model combustion chamber of a ramjet detonation engine was treated as a test. Geometrically, it is a hollow cylinder with the cylindrical internal body, which ends up as a cone. The fuel flow into the chamber through numerous injectors (premixed rich composition [H2]:[O2]=3:1, stagnant pressure 10 bar, stagnant temperature 258 K, Mach number at each orifice 1 (Fig1(1)). And from orifices with the flow perpendicular to the main flow (Fig1(2,3)) supplied only O2, stagnant pressure 15 bar, stagnant temperature 258 K. At the initial instance, the chamber is filled with air at 1 bar pressure and 300 K temperature. The ignition is made by means of an external energy source into a small spherical portion: rign =2.5 mm during the first tign=10-6 seconds from the initial instance, and with power per volume as high as Q=20 kW/mm3.

Fig. 1. The geometry of combustion chamber.

The species list and the kinetic mechanism: Hydrogen, oxygen and nitrogen were the initial and the inflow mixture components. In the process of combustion, besides the main product, water vapor, numerous products (radicals) are originated; at high temperature they still persist in the mixture, and at lower temperature they decay. We used the following set of species: {H2O, OH, H, O, HO2, H2O2; O2, H2, N2}. The research used a kinetic mechanism consisted of 20 reversible reactions. To direct the detonation wave, the gas mixture supply was not uniform at the beginning: the orifices opened gradually, depending on their angular coordinate.

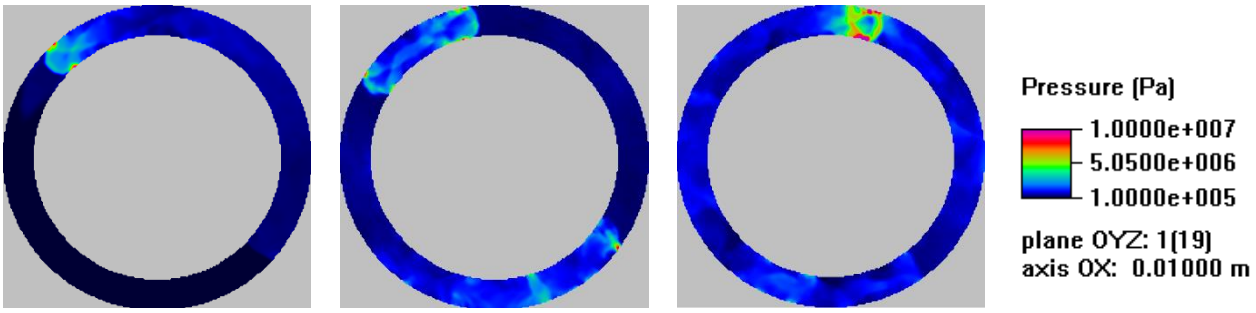
5 Numerical scheme

The calculations are based on the Navier – Stokes system of equations along with the equations for turbulence modeling and the chemical kinetics. The numerical modeling used the MUSCL interpolation of variables from the cells centers to the cell faces, together with the explicit AUSM-plus method stabilizing the scheme. The method was 2nd order both in space and time, except for tiny zones of strong gradients of

variables. The chemical kinetics containing 20 reversible elementary reactions with 9 species, was modified Maas – Warnatz, the reverse reactions kinetics was calculated using the equilibrium constant. The flux from chemical reactions was obtained semi-implicitly.

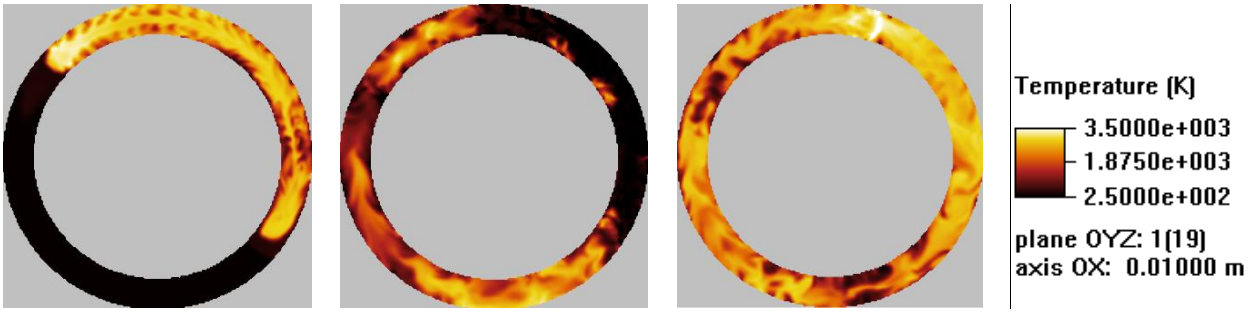
The computational domain used a regular mesh of uniform cubic elements. In the case under consideration, the work area contains more than 9 million cells. The time-critical program parts were parallelized using the OpenMP technique.

6 Results and Conclusions



a b c

Figure 2. Pressure in the cross section at various times on axis OX: a) t=50μs, b) t=200μs, c) t=850μs



a b c

Figure 3.Temperature in the cross section at various times on axis OX: a) t=50μs, b) t=200μs, c) t=850μs

As the Fig. 2-3 show, a strong detonation wave originates after the ignition; it propagates rotating between the coaxial cylinders in the front portion of the combustion chamber. After 100 μs, the system partially loses stability, and a secondary detonation wave starts originating. At 200 μs, the second detonation wave is moving directly towards the original one. For the rich mixture under consideration, a periodic "explosion in an explosion" takes place then, and this makes the original wave go galloping: fading and then re-originating .As the result of the numerical experiment, for the given parameter set, we obtained a galloping detonation wave rotating around the bottom of the combustion chamber. In the beginning, a stable detonation wave originates, but after 300 μs it splits into two, even 3 waves, which then join into a single detonation wave. After that, in some time the process repeats: lateral waves reflections from walls contribute to it.

Was received a galloping regime of detonation: a stable detonation wave originates, but after some time it splits into two, even 3 waves, which then join into a single detonation wave (the original wave fades, and a secondary wave increases). Such regimes are responsible to destabilize the work of a rotating detonation engine and should be avoided in practice.The case is not an optimal one from the thrust production and stability of burning point of view; it challenges to seek for more stable rotating detonation mode and parameters ensuring it. Yet the study of unstable modes of rotating detonation is still of a great value, as other transitional effects in combustion chambers.

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