Three dimensional numerical study of the propulsion system based on rotating detonation using Adaptive Mesh Refinement

Karol Swiderski, Michal Folusiak, Borys Lukasik
Arkadiusz Kobiera, Jan Kindracki, Piotr Wolanski
Institute of Aviation
Warsaw, Poland

Key words: detonation, CFD, AMR, hydrogen, RDE

1 Abstract

This paper presents the application of modern numerical methods and the technique of Adaptive Mesh Refinement (AMR) to the simulation of Rotating Detonation Engine (RDE) in three-dimensional space. The proposed numerical simulation model has been implemented into an in-house code REFLOPS USG.
Due to the limitation of computational resources only a large structure of the detonation wave is simulated. However the obtained numerical solution seems to be reasonably accurate in terms of the most important flow parameters of the detonative combustion chamber. A comparison to experimental data is provided either.

2 Role of numerical simulation in RDE project

Modern classical jet and rocket engines have almost reached a level of development where it is very difficult to improve their performance by minor modifications or just by improving the material parameters. In order to achieve significant increase in thermal efficiency of such engine some extraordinary steps must be applied, e.g. change of the thermodynamic cycle of the engine. This goal can be achieved by using detonation mode in RDE [1, 2] or Pulsed Detonation Engine (PDE). The detonation wave in RDE propagates continuously in an annular chamber. The engine is more compact and efficient. Smaller variations of thrust are created. Additionally, once initiated it propagates continuously. There is also a possibility of reducing NOx emission by use of lean mixtures which can burn at lower temperature compared to that obtained in stoichiometric region of combustion in classical burners.
Since the detonation is a combustion process in a constant volume, efficiency of the thermodynamic cycle is higher and there is potential to increase overall efficiency of the engine by order of 10%. The challenge in RDE project is realising the efficiency of the detonation cycle. Because the detonation wave propagates azimuthally around an annular combustion chamber, the kinetic energy of the flow can be held to a relatively low value and thus RDE may use most of the compression to increase the efficiency.
Nowadays rotating detonation has become a subject of numerical research at many institutions all over the world. The three-dimensional simulations performed by M. Liu et al [3] for premixed stoichiometric hydrogen-air mixture have uncovered some interesting properties of rotating detonation wave. The authors used one-step chemical kinetics model in their simulation model with a grid size lower than 0.5 mm. If the chamber depth was small the difference between the results at the inner and outer wall was not significant therefore in this case performing 2D simulations should be enough to obtain reasonable results. However, if the chamber height was

Correspondence to: karol.swiderski@ilot.edu.pl

larger, then the wave pattern was more complex in radial direction and only 3D simulations may be able to provide reliable results. Moreover it was also observed that chamber depth has no effect on detonation height as well as if the chamber depth was higher, the cycle period increased a little bit, and maximum pressure of the flowfield increased linearly.

The theoretical and computational aspects of RDE have been investigated in Japan by Yamada et al [4], and have been concerned with studying the limits of detonation operation. Hishida et al [5] have investigated the structure of detonation wave in RDE through detailed numerical analyses and have discovered Kelvin-Helmholtz instabilities and cell structures in RDE chamber. Some collaborative works have been also made by Hayashi et al in order to compare the numerical results with experiments performed by Polish researchers, Kindracki and Wolanski [6].

The main purpose of computational simulations performed by the authors of this paper is to provide fundamental results of RDE engine work. The results are an important part of the Innovative Economy project realised at the Institute of Aviation in Warsaw (2010-2013) and entitled 'Turbine engine with detonative combustion chamber'. An example of performed numerical analyses is presented in this paper.

The goal of the project of RDE engine is to develop an unique prototype of turbine jet engine equipped with detonative combustion chamber in place of a classical one. The detonative combustion chamber should utilise the effect of rotating detonation to produce the energy needed for the turbine.

3 Numerical method

The flow is modelled by Favre Averaged Navier Stokes Equations:

$$\frac{\partial}{\partial t}\int_V \underbrace{\mathbf{U}}_{\text{vector of conserved variables}} dV + \sum_{j=1}^{N_{faces}} \underbrace{\mathbf{T}}_{\text{transformation matrix}}^{-1} \int_{A_j} \left(\underbrace{\mathbf{F}^j}_{\text{vector of convective flux at face j}} - \underbrace{\mathbf{G}^j}_{\text{vector of diffusive (viscous) flux at face j}} \right) dA_j = \int_V \underbrace{\mathbf{H}}_{\text{viscous source term for k-}\varepsilon\text{ model}} dV + \int_V \underbrace{\mathbf{S}}_{\text{source term for chemistry, injection etc.}} dV$$

The model employs HLLC Riemann solver [7] for semi-ideal gas with chemical reactions. Explicit Euler scheme is used to integrate the flow in time and implicit DVODE solver [8, 9] for chemical equations as well. Additionally 2-stage AMR technique is used in the simulation. To simulate inflow and outflow environment conditions compressible boundaries are employed: pressure inlet and pressure outlet boundary conditions for both subsonic and supersonic flows. Wall viscous effects are neglected therefore the slip walls are assumed. Furthermore the standard k-ε model of turbulence is used to describe the formation of the hydrogen-air mixture nearby injection zone. The details of implementation technique into the REFLOPS USG code [10, 11] are omitted in this paper.

4 Chamber geometry and discretization

The mesh consists of 187072 hexahedral elements with minimum cell size of 2.2 mm. Using 2-stage AMR reduced the minimum cell size to 0.55 mm. The meshed geometry is presented below in Fig. 1:

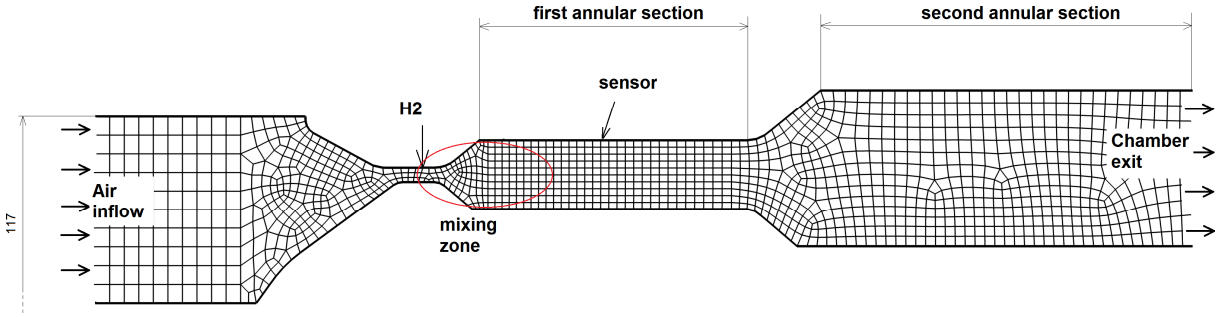

Figure 1. Chamber geometry sketch. 2D cross section with mesh.

The geometry was separated into two annular chambers because it has been designed for hydrogen and JET-A detonation. The first has a height of 22 mm, the second 50 mm. In the first section a hydrogen-air detonation wave was expected to propagate while in the end part of the chamber a JET-A and air detonation was to occur.

However a JET-A and air detonation is omitted here, and the end part of the chamber is treated as expansion section. Hydrogen injection was realised by 90 numerical injectors with 0.7 mm diameter placed perpendicularly to the flow direction as shown above. There was also static pressure numerical sensor located at the outer wall of the chamber.

5 Chemical mechanism

Some efforts have been undertaken to find the optimal chemical mechanism. There is a wide choice of hydrogen – air combustion mechanisms presented in literature. The level of details ranges from global reaction to detailed reactions with hundreds species. In the presented simulations the numerical cost was the driving factor and a single-step global reaction mechanism was chosen:

$$2H_2 + O_2 = H_2O + H_2O \qquad E_a = 1.2\text{e}4 \text{ cal/mole} \qquad n = 0 \qquad A = 2e17 \text{ [mole,cm,s,K]}$$

This mechanism was checked against the Petersen 21-step mechanism [12] in case of 1D simulation of propagating detonation wave. Fig. 2 demonstrates that the differences between results of both mechanisms are relatively small. The discrepancies manifest mainly in the vicinity of the leading shock and vanish in farther distance from the shock. This should not be a problem while only large scale is simulated here. Additionally, the simple mechanism enables 4 to 5 faster calculations for 1D simulations.

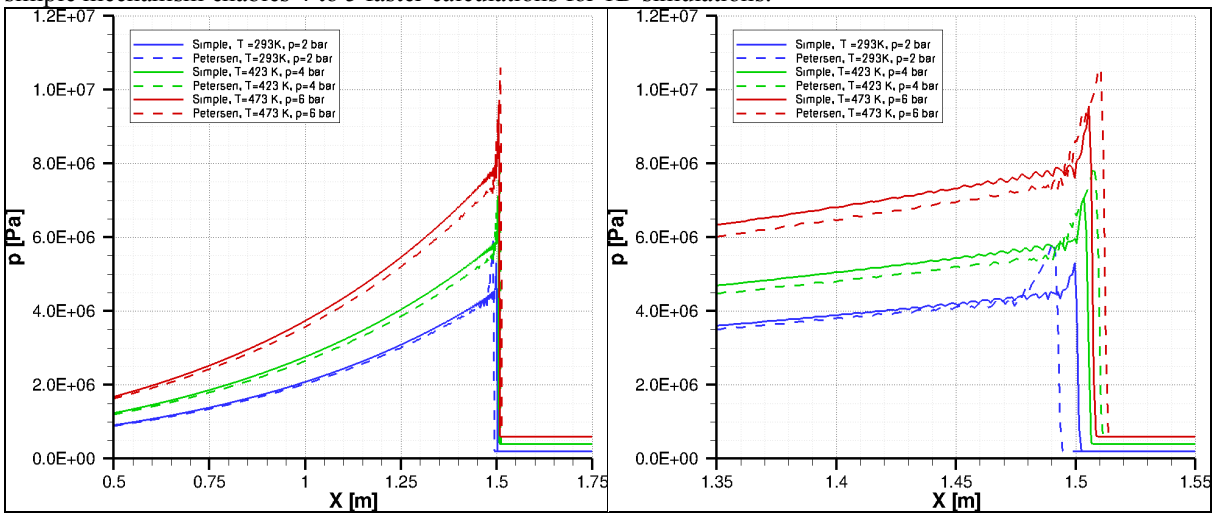

Figure 2. Comparison of chemical reaction mechanisms: simple and Petersen. Left: wide X range. Right: zoom nearby pressure peak.

6 Simulation procedure and results

Before the detonation is initiated the goal is to obtain a steady state solution of air flow with fuel injection. From that analysis a height of mixture layer can be found and since the present numerical model is non-premixed one can expect that there will be non-uniform profile of mixture composition where the detonation wave propagates, as shown below in Fig. 3. In this case there is a wide zone of stoichiometric mixture which corresponds to y_H2=0.0282. The mixture layer width for $\phi \simeq 0.5 \div 1$ equals about 2/3 of channel height, the mixture is more fuel rich close to the outer side due to injectors location.

In the simulation of RDE the initiation process must be conducted carefully. In reality the time of establishing of stable rotating detonation lasts about a few hundreds of microseconds or even longer. The initial chaotic state of the waves was obtained both in experiments and calculations [13; 14]. Simulation of this transition would be prohibitively long for the 3D simulations. Therefore the initiation of the wave must be artificially triggered in order to get quickly the stable rotating wave. The ignition of hydrogen-air mixture is accomplished by a simulated spherical igniter here. At the beginning of ignition process only a half of the chamber is activated for chemical reactions. In the rest of the computational domain chemical reactions are switched off. When the detonation wave reaches approximately 40% of circumference of the chamber the second half of the chamber is activated for chemical reactions. This methodology allows avoiding creating two detonation waves propagating in two opposite directions during the ignition.

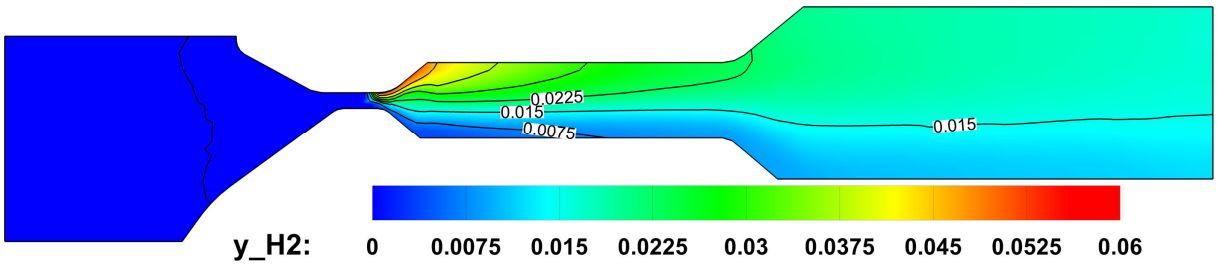

Figure 3. Mass fractions contours of hydrogen. 2D cross section. Note: The scale upper limit denotes $\phi \approx 2$.

The quasi-state solution was obtained without using of AMR. Then the mesh was adapted by pressure gradient criterion (for the refinement 35e6, derefinement 25e6 Pa/m). It should be also noticed that for AMR constant massflow injectors were used instead of constant pressure type as in the simulation for the fixed grid. At the outlet of the chamber the normal conditions were assumed.
Numerically calculated static pressure is compared to experimental data and averaged flow parameters are presented below in Fig. 4 and Tab. 1:

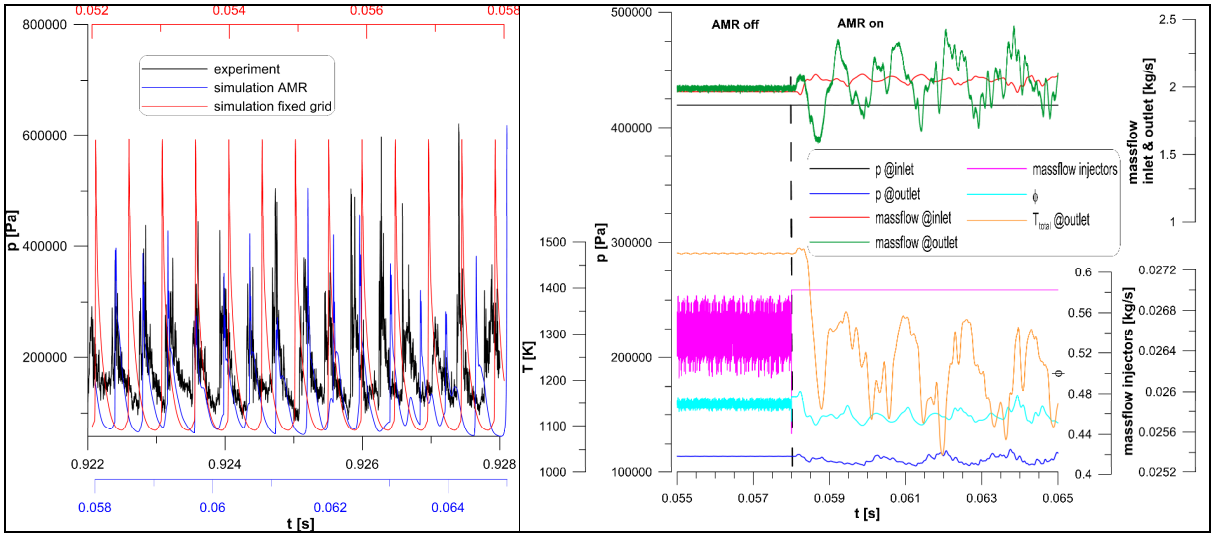

Figure 4. Flow parameters. Left: Pressure history. Right: Averaged flow parameters from the simulation.

Table 1. Comparison between simulation and experiment.

	Simulation (AMR)	**Simulation (fixed grid)**	**Experiment**
Inlet total pressure [bar]	4.2	4.2	4.217
Inlet total temperature [K]	420	420	390
Mixture equivalence ratio ϕ	0.45-0.48	0.47	0.49
Outlet total temperature [K]	1050-1350	1470	1089
Inlet air massflow [kg/s]	2±5%	2	2.001
Detonation velocity [m/s]	1351	1259	1605 (FFT analysis)
Detonation temperature [K]	1800-1900	1790	1850

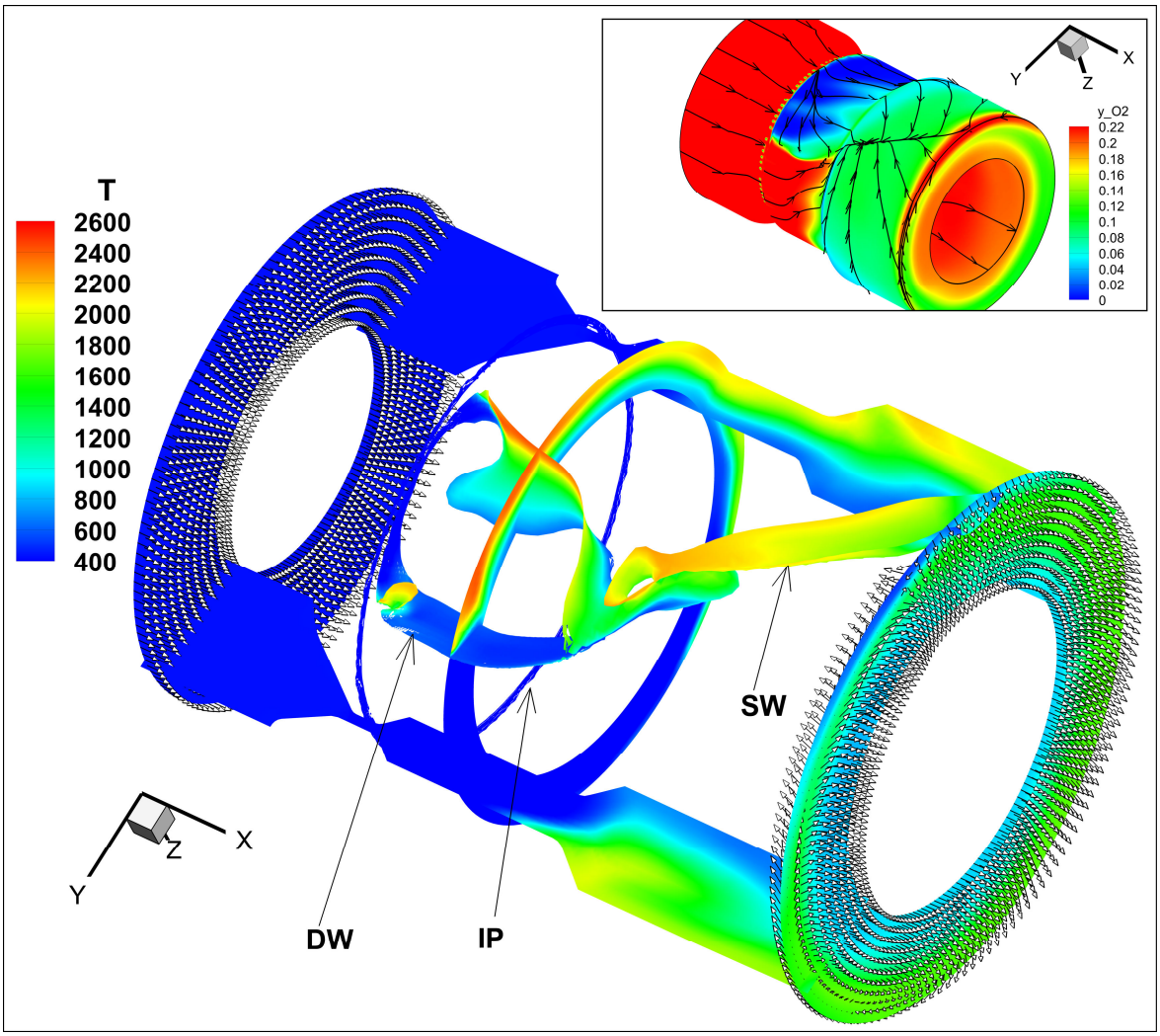

Figure 5. Detonation wave propagation. Main frame: Large scale structure of the detonation wave (DW) as an isosurface of pressure equal 0.2 MPa. Distribution of velocity vectors at the inlet at outlet section of the chamber. Each surface is coloured by static temperature contours [K]. A slice in the central part of the chamber is coloured by static temperature contours either. SW is a shock wave propagating downstream, IP denotes injection plane location. Right upper corner: Streamtraces of the flow. Contours of oxygen mass fractions.

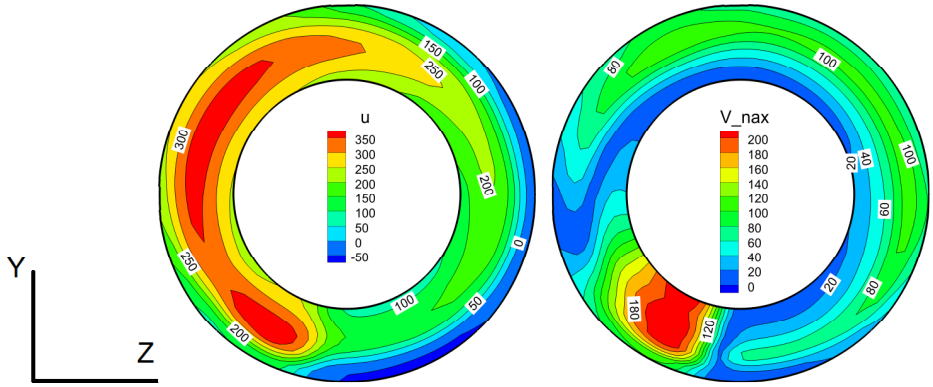

Figure 6. Contour map of axial (u) and non-axial (V_nax) velocity at the outlet section of the chamber [m/s].

7 Conclusions

Quite similar profile of pressure peaks was obtained both in the simulation with AMR and experiment. A little bit higher detonation velocity (1605 vs. 1351 m/s) is observed in experiment. This is probably due to the fact that in the experiment a non-uniform mixture and its composition can change significantly in time. As far the detonation wave obtained in the simulation with AMR, it has a reasonable speed (about 15% lower than C-J velocity of 1582 m/s). An interesting observation is that after AMR was activated a noticeable effect on outlet temperature can be observed. First it is closer quantitatively to the experimental data (1089 K, measured by thermocouple placed at 5 mm radial distance from the outer wall at chamber exit) than it was before. Moreover a regular temperature oscillations are observed at the outlet plane, within a range of 1050-1350 K. It is also worth to mention that the massflows at the inlet and outlet started varying. Generally the velocity profile at the air inlet is uniform, but at the chamber exit a wide region of backflow is created. It has been shown in Fig. 5 that this backflow occurs close to the outer wall and spreads over about 1/3 of outlet circumference. The shock wave (SW) divides the region of backflow and swirled flow in the second annular section of the chamber as shown in the right corner of Fig.5. The flow is almost parallel to the X axis in about 1/4 of outlet area, see Fig. 6. The mass weighted average of velocity components u, v, w at the outlet equal 195, 33.5 and 33 m/s respectively. Therefore a relative difference between mean radial and axial velocity is about 17%. Generally it has been observed that the results obtained using AMR are qualitatively much closer to the real data than from classical simulation on a fixed grid [14], even for such simple chemical mechanism as here. Furthermore the authors observed that AMR utilization enables resolving the flowfield in RDE more precisely and allows reducing CPU time by half.

Acknowledgements

This work was conducted in frame of project UDA-POIG.01.03.01-14-071 'Turbine engine with a detonation combustion chamber' supported by EU and Ministry of Regional Development, Poland.

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