Assessment of numerical simulations of RDE combustion chamber

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1 Abstract

The paper presents results of three-dimensional numerical simulations of a H_2 -air detonation combustion chamber. Results are compared with experimental data for the combustion chamber of turboshaft RDE engine investigated at Institute of Aviation in Warsaw. Authors prove that even very simple models, of inviscid, premixed gas mixtures can be successfully used in detonation simulations and in preliminary performance assessment. The assessment of the three approaches to modelling of combustion chamber of the RDE was performed. The study has been conducted on very simple model of inviscid flow with premixed mixture and two more sophisticated and computationally expensive models of inviscid or viscous flow with numerical injectors.

2 Introduction

The Rotating Detonation Engine (RDE), also known as the Continuous Detonation Wave Engine, is the next to the Pulse Detonation Engine most commonly considered propulsion system utilizing the detonation wave. The principle of the RDE operation is based on the continuous propagation of spinning detonation wave in disk-like or annular chamber.

The most commonly listed advantages of the RDE are due to the very fast energy release during the detonative combustion. The combustion zone is smaller than in the deflagration, thus the chamber can potentially be shorter. Another consequence is that the combustion process is thermodynamically closer to a constant volume process which is more efficient than the process of constant pressure, typical for a conventional air-breathing propulsion system. According to the comparison made by Kindracki [1], for stoichiometric mixture of hydrogen and air, thermodynamic efficiencies are 59%, 54% and 37% for the detonation, constant volume, and constant pressure cycles respectively, assuming the adiabatic compression is 5 for each cycle. Another possible advantages of the RDE over state-of-the-art air-breathing jet engines are low NOx emissions and the simplicity of the construction [2].

Nowadays, many laboratories over the world conduct their experiments on the rotating detonation and the RDE [2][3]. In Poland experimental works are conducted at Institute of Heat Engineering of Warsaw University of Technology and from 2010 also at Institute of Aviation. The latest result of cooperation of these two institutes is the project started in 2010 in the framework of Operational Programme Innovative Economy entitled "Turbine engine with detonation combustion chamber".

Parallel to the experimental group, the numerical group has been established. Researchers are developing numerical tools that are necessary for simulations of processes being investigated. Codes that have been

validated with the experimental data can be further used as a cheap alternative for experiments or for better understanding of processes with wider range of parameters that are hardly available from experimental results.



Figure 1. Left: Turboshaft Rotating Detonation Wave Engine. Right: Geometry of the combustion chamber of the RDE. The main flow direction is from left to right.

Numerical simulations are useful as long as results can be obtained in reasonable time. It is therefore of advantage to simplify numerical models used in order to shorten the simulation time. On one hand, it is of practical significance to take the methods of mixture creation and viscosity of gas mixture into consideration in the RDE simulations since fuel and oxidizer are usually delivered to the RDE chamber in separate streams. On the other hand, the model based on Euler equations is currently accepted and widely used in many scientific publications. The purpose of presented work is to investigate the influence of the modelling approach used on basic parameters of the RDE operation. The comparison presented below is not intended to discuss the details of accuracy of any of presented models since at the stage of preliminary design of the RDE chamber only qualitative agreement between experimental and numerical results is expected.

This work presents results of three-dimensional simulations of the detonation propagation in candidate combustion chamber of the turboshaft RDE engine shown in Fig. 1, which is the subject of the aforementioned project. Experiments are performed on both H_2 and Jet-A, results of H_2 -air detonation are presented below.

3 Mathematical and numerical model

Simulations presented in this paper are based on the Reynolds Averaged Navier-Stokes equations, extended to describe the motion of a multicomponent reacting gas, discretized on unstructured grid, in the form:

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

Numerical fluxes \mathbf{F} are evaluated with HLLC approximate Riemann Problem solver [4]. Convective and diffusive terms are integrated in time by use of the explicit Euler method. In case of viscous flow, the standard k- ε turbulence model is used and wall viscous effects are neglected. The model is used for modeling of H₂-air mixture formation near injection zone. If the inviscid flow is considered, the equation presented above simplifies to Euler equations for multicomponent reactive gas. The source term \mathbf{S} is chemical composition change rate resulting from the chemical reactions. The production rate of chemical compounds is an overall sum of the production and destruction rates for a given chemical compound in all reactions taken into account in the chemistry model. The chemical reaction sources are integrated by the quasi-equilibrium solver DVODE [5]. The model is implemented into the in-house code REFLOPS USG [6,7].

In the particular case presented in this work, combustion of hydrogen is described by one reversible reaction. The forward reaction rate is calculated by use of classical Arrhenius equation with the reaction rate constants verified against the Petersen 21-step mechanism [8] for the case of one-dimensional detonation propagation. The

backward reaction rate is calculated from the assumption of local chemical equilibrium. The global mechanism can be written as follows:

$$2H_2 + O_2 = H_2O + H_2O$$
 $E_a = 1.2e4\frac{cal}{mole}$ $n = 0$ $A = 2e17(mole, cm, s, K)$

4 Computational model of the RDE chamber

The combustion chamber of the RDE investigated at Institute of Aviation consists of two annular sections of heights 22 and 50 mm (see Fig. 2). The injection of gaseous hydrogen is realized with 90 orifices of 0.7 mm diameter, placed perpendicularly to the flow direction at the inner surface of throat. Pressure sensor is placed at the outer surface, in the middle of the first section.

The computational model of the stepped chamber was build up from 190 000 hexahedral elements, the smallest element size is 2.2 mm. Numerical sensors and injectors are placed at positions corresponding to positions of real devices. In case of premixed computations and when no mixing model is used, it is of advantage to suppress chemical source terms in detonation simulations in certain subdomains of computational model. Such manipulation can be used to imitate the mixing length. In Fig. 2 it is shown that in presented case the chemical reaction can occur only downwind the first divergent section.



Figure 2. Longitudinal section of computational model of the RDE geometry.

5 Results

The assessment of three approaches to modelling of combustion chamber of RDE was performed. The study has been conducted on: model of inviscid flow with premixed gas mixture; model of inviscid flow with numerical injection of hydrogen and model of viscous flow with numerical injectors and the standard k-e turbulence model.



Figure 3. Comparison of pressure profiles on sensors.

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Results of the three approaches are compared to results of experimental investigation. In all investigated cases the chamber inlet pressure was 4.2 bar and the mean air-fuel equivalence ratio λ was about 2. The pressure at chamber outlet was 1 bar. In Fig. 3 comparison of pressure profiles for 3 approaches and experimental data is shown. The resulting working frequency in each simulation is very similar and much lower than measured during experimental research. This observation is confirmed by measurements of detonation wave speed, shown in Tab. 1. The linear wave speed measured along the mean circumference (0.635 m) almost exactly matches the C-J velocity, which is 1582 m/s in this case. Pressure peaks are higher than in experiment in case of inviscid and viscous injection, and even higher in case of premixed gas.

In Fig 4. the comparison of the flow field near the detonation wave is presented. The mixture composition differs significantly between models, however the shape of rotating detonation wave and location of other waves is similar. The details of the mass fraction distribution and the flow field obtained with viscous model can be found in separate paper [9].



Figure 4. Isosurfaces of static pressure; isolines of density and contours of mass fraction of H_2 shown at the surface of mean chamber diameter. Results of (a) inviscid premixed, (b) inviscid and (c) viscous with injection simulations. The main flow direction is from up to bottom.

In Tab. 1 also temperature measurements available from both the experimental and numerical investigations are presented. Since the overall time of experiment (several seconds) was too short for thermocouple to reach the equilibrium temperature, the approximation of the transmittance of thermocouple with a second order inertial term was used to approximate the actual temperature. However, the results obtained with use of any proposed numerical models differ significantly from experimental one.

The results of the three investigated models shown in table below are supplemented by the results obtained for premixture with use of Adaptive Mesh Refinement (AMR). The technique was used in order to check the convergence of selected numerical method. Results of solutions with doubled spatial resolution are presented in table. It is shown, that for two times finer mesh the temperature and wave speed are much closer to experimental data than results of any of the models used on coarse mesh. Pressure peaks are however much higher which is due to lack of viscous losses.

Thrust F and fuel-based specific impulse ISP_{f} are evaluated according to the following equations:

$$F = \int (\rho u^2 + p - p_{\infty}) dA \qquad ISP_f = \frac{F}{g\dot{m}_f}$$

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where ρu^2 and p are normal momentum and pressure at chamber exit, p_{∞} is ambient pressure, g and \dot{m}_f are gravity acceleration and fuel mass flow rate respectively. Results of specific impulse measurements are very promising and in case of inviscid computations shown in Tab. 1 are all in range 4550-4750 s. In case of RANS simulations the value of specific impulse is considerably reduced by viscous losses.

	Air-fuel	Mass			Mean	Specific
	equivalence	flow rate	Temperature	Wave	pressure	impulse
	ratio	at outlet	at outlet	speed	peak	ISP_{f} [s]
Case	λ[–]	[kg/s]	[K]	[m/s]	p _{peak} [bar]	4
Experimental	2.05	2.0	1198	1605	5	N/A
Simulation, viscous, injection	2.13	2.0	1450	1258	6	4040
Simulation, inviscid, injection	2.08	2.1	1341	1143	6	4550
Simulation, premixed, base grid	2.00	1.9	1345	1243	7	4670
Simulation, premixed, fine grid	2.00	1.9	1240	1354	7.5	4750

Table 1. Comparison of detonation parameters.



Figure 5. Results of the RDE simulations for model of inviscid flow with premixed mixture. (a) Contours of pressure at selected sections; contours of (b) temperature, (c) pressure, (d) axial velocity and (e) non-axial velocity magnitude and vectors at outlet section.

In Fig. 5(a) the pressure field at selected sections of combustion chamber is shown. The region of the highest pressure lies in the middle of first annular section and at the outer surface of the chamber. In Fig. 5(b-e) the

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influence of the shock wave entailed by the detonation wave on the uniformity of outlet parameters is demonstrated. Relatively high pressure can be observed at the outer surface of combustion chamber, while the temperature is distributed more uniformly. The highest axial velocity of 500 m/s is observed in the middle of channel height after the shock wave. The axial velocity before the wave is relatively small and backflow not greater than 50 m/s is observed near the outer surface. The flow after and before the detonation wave is the more circumferential the closer the wave is. The circumferential velocity component dominates the non-axial velocity, and radial component is relatively small.

Irrespective of the results presented above, it can be shown that mean axial velocity and mean velocity magnitude at outlet differ by less than 5%. The instantaneous results shown in Fig. 5 are not of practical importance in terms of performance. Since the work frequency of the RDE is of order of several kHz, it may be said that the flow is nearly axial. However, the presence of high velocity gradients and shock wave at outlet section must be kept in mind.

6 Summary

Similar profiles of pressure peaks have been observed in case of each investigated models. The perfect agreement of detonation velocity measured experimentally with C-J velocity has been shown, while for each of the investigated models the detonation propagation velocity was slightly lower. Similar observations have been made in case of computed outlet temperature which was higher than temperature measured experimentally.

These discrepancies can be justified by relatively coarse mesh (minimum cell size 2.2 mm) which was a compromise between an acceptable accuracy and performance required during the preliminary design process. When finer mesh was used, results much closer to experiment were obtained, what proves that selected model of detonation propagation is appropriate.

The purpose of presented work was to investigate the influence of the modelling approach on basic parameters of the RDE operation that are of interest during the preliminary design process. In this paper, it has been briefly demonstrated that in such case relatively simple methods based on Euler equations can be successfully used in detonation simulations and in preliminary performance assessment.

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