## Mathematical modeling of detonation initiation via flow cumulation effects

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Theoretical studies of gaseous detonation initiation via flow cumulation effects and relatively weak shock waves convergence were started in 1970-s in the works of V.P. Korobeinikov, V.A. Levin, V.V. Markov etc. In author's findings [1, 2] the novel method for shock-todetonation transition (SDT) due to the special plane or axisymmetrical tube walls profiling was introduced and investigated. The mechanism of initiation was determined by the gas dynamics cumulation effects when the initiating shock wave (ISW) interacted with the profiled walls. The stoichiometric propane-air mixture was considered. These results were followed by considering of essentially three-dimensional (3D) tube geometries – tube coils [3] and helical tubes [4].

The paper concerns two problems. The first one is 3D numerical investigation of SDT in stoichiometric methane-air mixture under normal conditions in a tube with parabolic contraction, connecting section of narrow diameter and conical expansion. Investigation of detonation initiation critical conditions for natural gas-air mixtures is very important and promising problem from the sense of development pulse-detonation engines. The shape of parabolic contraction and divergence angle of cone expansion are found which provide SDT for the ISW Mach number about 3.3. The results of 3D numerical investigation confirm in whole the results of previous two-dimensional (2D) findings. At the same time in 3D calculation the realistic three-dimensional detonation irregular cellular structure is obtained which couldn't be obtained in 2D axisymmetrical study (see Fig. 1). It is demonstrated, that there are different regimes DW propagation in conical expansion.



Fig. 1. Comparison of "numerical soot footprints" in 2D and 3D calculations of the methane-air detonation initiation problem

The second problem is numerical study of the start-up of the small-scaled hydrogen electrochemical pulse detonation engine model with the use of electrical discharge which causes the toroidal shock wave in the vicinity of chamber walls. The parameters of the engine are taken from [5]. All the calculations are performed with the use of author's original software [4]. The chemical kinetics model includes 17 elementary reversible reactions [6]. The computational domain consists of combustion chamber only without inlet and outlet sections of the engine. The computations are performed on a grid with enough spatial resolutions about 0.015 - 0.02 mm. The total cells number is about 12.5 mln. The computations are performed in 3D statement in a sector with one cell in angular direction. The different combustion modes in chamber are investigated against electrical discharge energy -3, 6, 7, 8 and 10 J. As one can see on Fig. 2a for the discharge energy of 6 J the blast wave cumulation provides local explosion on the combustion chamber axis of symmetry in contrast to the case of energy 3 J, but the explosion is not strong enough to form detonation wave. Fig 2b demonstrates that the energy of 10 J is enough for direct detonation initiation on axis of chamber and the detonation wave doesn't decay while its propagation to the chamber walls. The detonation is overdriven with detonation cell size significantly smaller than the known experimental data.



(a) discharge energy 6 J, time moment 72  $\mu$ s



**Fig 2.** (a) Temperature distribution in Kelvin degrees and (b) "numerical soot footprints" for the problem of start-up of electrochemical pulse detonation engine model. Spatial scale in meters.

## References

1. Frolov S.M. et al. (2007) Reduction of the deflagration-to-detonation transition distance and time in a tube with regular shaped obstacles. Dokl. Phys. Chem. 415: 209-213.

2. Semenov I.V. et al. (2009) Numerical Simulation of Detonation Initiation in a Contoured Tube. Comb., Expl., and Shock Waves. 45, 6: 700-707.

3. Frolov S.M. et al. (2009) Shock-to-detonation transition in tube coils // Proc. 26th Int. Symp. Shock Waves. V. 1. Springer Verlag. 365-370.

4. Semenov I. et al. (2011) Three-dimensional numerical simulation of shock and detonation waves propagation in tubes with curved walls. Sci. Tech. Energ. Mater. 72, 4: 116-122.

5. Korobeinikov V.P. et al. (2001) Electrochemical Pulse Detonation Engine. High-Speed Deflagration and Detonation. Moscow: ELEX-KM Publishers. 289-302.

6. Pitz W.J. et al. (1984) A Comprehensive Chemical Kinetic Reaction Mechanism for the Oxidation of N-butane. 20th Int. Symp. Comb. 831-843.