EXPERIENCE IN NUMERICAL SIMULATION OF A METHANE–AIR MIXTURE TURBULENT COMBUSTION IN A DUCT WITH A STEP USING THE COMPUTATIONAL FLUID DYNAMICS PACKAGE ANSYS FLUENT ON THE BASIS OF VARIOUS CHEMICAL KINETICS MODELS

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Abstract: The mode with stabilization of premixed methane–air combustion in a subsonic flow in a duct with a backward step, which was studied experimentally in ONERA (Magre, *et al.*, 1988), is considered. Numerical simulation of this flow based on unsteady Reynolds equations was performed using the commercial computational fluid dynamics package ANSYS FLUENT. It is shown that using FLUENT, it is possible to achieve a solution quality comparable to the best results obtained at TsAGI using the in-house zFlare code. An example is presented when, at the use of turbulence–combustion interaction models in the calculation, the transition to a more detailed kinetic scheme led to a deterioration in the flow modeling quality compared to simplified kinetic schemes and an explanation of this result is given.

Keywords: subsonic premixed combustion; unsteady RANS; turbulence–combustion interaction; kinetic scheme; numerical simulation; experimental validation

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Figure Caption

Figure 1 Geometry of the computational domain (*a*) and grid in the vicinity of the step (*b*)

Figure 2 Vertical profiles of parameters at the entrance to the computational domain: (*a*) longitudinal velocity u; (*b*) turbulence intensity $\mathrm{Tu} = \sqrt{2k/3}/u_{\max}$; and (*c*) characteristic frequency of large-scale turbulence $e/k = 0{,}09w$

Figure 3 Vertical profiles of the average longitudinal velocity u in the calculation of the flow without combustion in three cross sections of the channel: (*a*) $x = 0.04$ m; (*b*) 0.10; (*c*) $x = 0.25$ m; *1* — experiment P. Magre *et al.*; *2* — FLUENT with SST model; *3* — CEDRE with k–l model; and *4* — zFlare with q–ω model

Figure 4 Mean temperature fields obtained in calculations: (*a*) SST, without TCI, Frolov4 kinetics; (*b*) Baseline k–ω, without TCI, Frolov4 kinetics; (*c*) Baseline k–ω, PaSR with $C_\tau = 0.11$, Frolov4 kinetics; and (*d*) Baseline k–ω, without TCI, Smooke25 kinetics

Figure 5 Comparison of vertical profiles of mean temperature (*a*) and longitudinal velocity (*b*) for different values C_τ (*1* — $C_\tau = 0.100$; *2* — 0.110; *3* — 0.120; and *4* — $C_\tau = 0.128$) with experiment (*5*): left column — $x = 0.10$ m; middle — 0.25; and right column — $x = 0.34$ m

Figure 6 Comparison of vertical profiles of average temperature (*1* — quasi-laminar calculation (without TCI); *2* — PaSR with $C_\tau = 0.11$; and *3* — EPaSR [30]) with experiment (*4*): (*a*) $x = 0.04$ m; (*b*) 0.10; (*c*) 0.15; (*d*) 0.25; (*e*) 0.34; (*f*) 0.46; (*g*) 0.71; and (*h*) $x = 0.91$ m

Figure 7 Comparison of vertical profiles of average longitudinal velocity (*1* — quasi-laminar calculation (without TCI); *2* — PaSR with $C_\tau = 0.11$; and *3* — EPaSR [30]) with experiment (*4*): (*a*) $x = 0.04$ m; (*b*) 0.10; (*c*) 0.15; (*d*) 0.25; (*e*) 0.34; (*f*) 0.46; (*g*) 0.71; and (*h*) $x = 0.91$ m

Figure 8 Comparison of three chemical kinetic mechanisms (*1* — BFER2; *2* — Frolov4; and *3* — Smooke25): (*a*) laminar flame distribution rates at different values of the fuel-to-air equivalence ratio in comparison with experimental data [40]; (*b*) dependence of temperature on time during combustion in the reactor ($p = const$); (*c*) dependence of the formation rate of water vapor on temperature corresponding to Fig. 8*a*; and (*d*) similar dependence corresponding to Fig. 8*b*

Figure 9 Heat release rate fields and longitudinal velocity isolines obtained in calculations based on the PaSR model using various kinetic schemes: (*a*) BFER2; (*b*) Frolov4; and (*c*) Smooke25

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