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Application of reactingCentralFOAM for Modeling Processes in Combustion Test Chamber

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Abstract. Features of numerical simulation of multicomponent reactive mixture flows using the OpenFOAM package reactingCentralFoam solver are considered. The specifics of the construction of the project on the basis of the calculation of the combustion of the oxygen-hydrogen mixture for the conditions of the experimental setup "Penn State Pre-burner Combustor" are discussed. The results of computations of the main parameters of the combustion process are given, the efficiency of the applied solver is shown.

INTRODUCTION

The computational gas dynamics is widely used in the design process of different technical devices, allowing to use difficult physical and mathematical models. In addition, the results of computations can be applied to the interpretation and better understanding of the operation of experimental installations. The mixing of fuel and air, self-ignition and flame stabilization are thus critical processes to understand and control different kind of devices: fuel-injectors, turbofan engines, supersonic combustion ramjets and scramjets.

The OpenFOAM library allows to use a set of the solvers realizing specific models for turbulent flows [1]. The OpenFOAM library on the structure and flexibility can be quite selected as a basic code for simulation of compressible reacting gas flows in combustion chambers for different engines [2-4]. The family of solvers was developed for simulation of flows in a wide range of Mach numbers in ISPRAS [5]. In particular, the solver reactingCentralFoam was developed for computation of flow for reacting mixture. The goal of this study is computation and assessment simulation's results of the known test example "Penn State Pre-burner Combustor" [6].

DESCRIPTION OF THE EXPERIMENTAL SETUP

Experimental chamber assembly, shown in Fig. 1 and 2, consists of preliminary burners, a coaxial injector, a main combustion chamber, a chamber for measuring the wall and heat flow temperature, and a water-cooled nozzle. The oxidizer (oxygen) is fed into the combustion chamber through the inner tube of a coaxial injector with a diameter of 5.26 mm and recessed by 0.43 mm relative to the combustion chamber face. The annular hydrogen supply has an internal diameter of 6.30 mm and an outer diameter of 7.49 mm. In the inlet section of the oxygen tube are known: pressure 5.85 MPa, temperature 711 K, mass flow rate 0.0904 kg / s, mass concentration of the mixture - oxygen 0.945, water 0.055. In the inlet section of the fuel ring: pressure 6.5 MPa, temperature 800 K, flow rate 0.0331 kg / s, mass concentration of the mixture - hydrogen 0.402, water 0.598. The measured pressure in the main chamber was 5.17 MPa or 750 psia.

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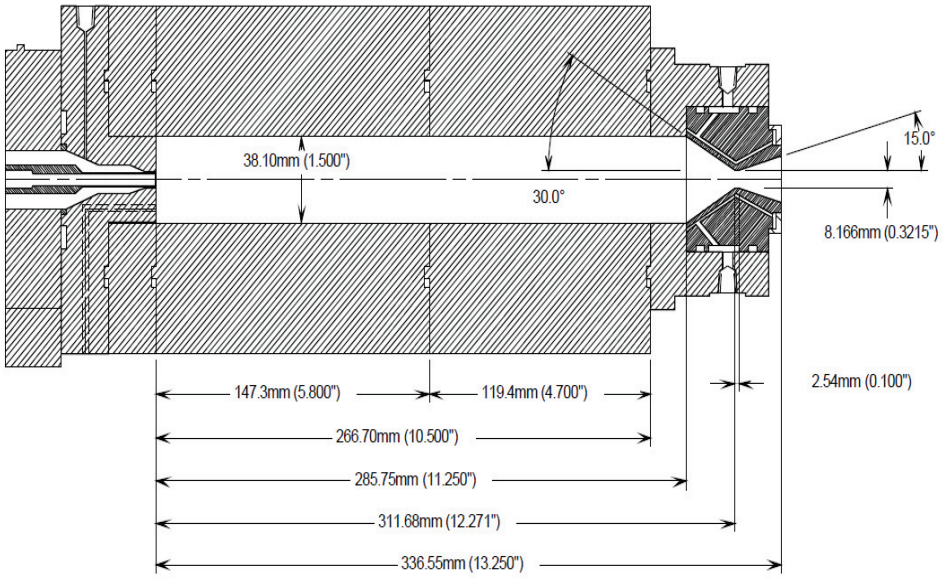

FIGURE 1. Schematic of integrated pre-burners/main

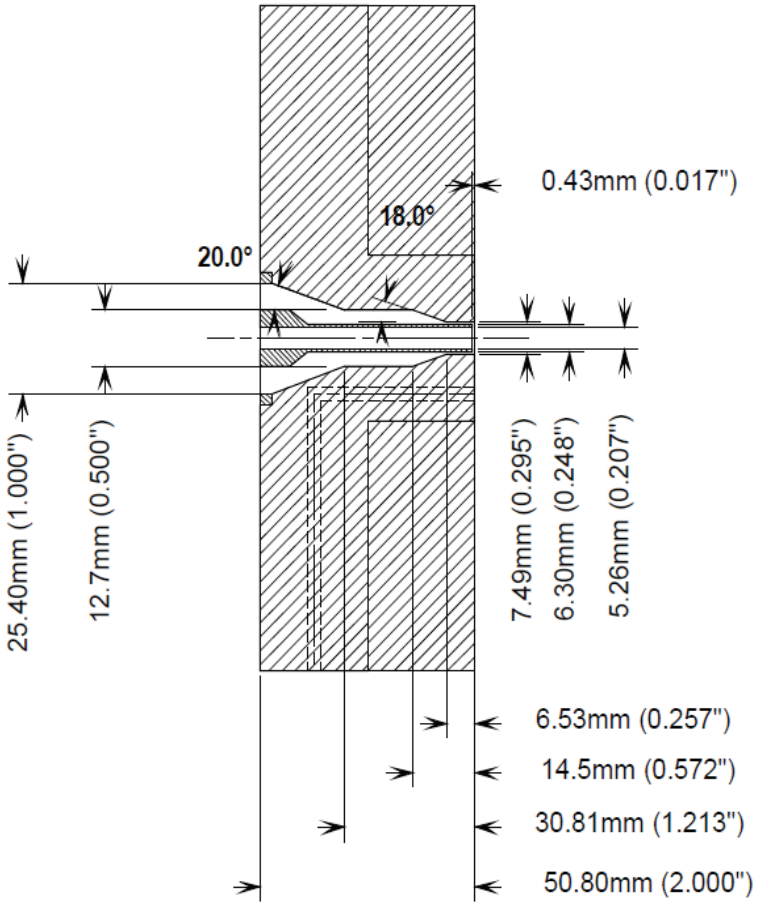

FIGURE 2. Shear coaxial injector

MATHEMATICAL FORMULATION AND PARAMETERS OF A NUMERICAL MODEL

The system of equations

The gas flow mixture is described by the continuity equations, momentum and energy equations written for compressible, viscous, heat-conducting, reacting gas with k-ω SST turbulence model and also continuity equations for each components of mixture. The system of equations is shorted by an equation of state for ideal gases, the caloric equation, formulas for computation of viscosity, heat conduction, a heat capacity. All numerical computations are performed using second-order accurate numerical schemes in space. The model of chemical kinetics using 9 components and 23 chemical reactions is applied to a case with burning hydrogen and oxygen [7].
The reaction rates are determined by laminar finite-rate model [8, 9].

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\frac{\partial (\rho h_s)}{\partial t} + \frac{\partial (\rho h_s u_j)}{\partial x_j} + \frac{\partial (\rho K)}{\partial t} + \frac{\partial (\rho K u_j)}{\partial x_j} - \frac{\partial P}{\partial t} = \frac{\partial (u_i \tau_{ij})}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\chi \frac{\partial h_s}{\partial x_j}\right) - \sum_{m=1}^{N} \frac{\partial}{\partial x_j}\left(\chi h_{s,m} \frac{\partial Y_m}{\partial x_j}\right) - \sum_{m=1}^{N} \frac{\partial}{\partial x_j}\left((\mu + \right.$$

$$\left. + \mu_t) \frac{\partial Y_m}{\partial x_j} h_{s,m}\right) + S_{hc}$$

$$\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left((\mu + \sigma_K \mu_t) \frac{\partial k}{\partial x_j}\right) + \tilde{P}_K - \rho \beta^* k \omega$$

$$\frac{\partial (\rho \omega)}{\partial t} + \frac{\partial (\rho \omega u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left((\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_j}\right) + \alpha \rho S^2 - \rho \beta \omega^2 + (1 - F_1) 2 \rho \sigma_{\omega 2} \frac{1}{\omega} \frac{\partial \omega}{\partial x_j} \frac{\partial k}{\partial x_j}$$

$$\frac{\partial (\rho Y_m)}{\partial t} + \frac{\partial (\rho Y_m u_j)}{\partial u_j} = \frac{\partial}{\partial x_j}\left((\mu + \mu_t) \frac{\partial Y_m}{\partial x_j}\right) + \omega_m \quad m = 1 \ldots N - 1 \quad \sum_{m=1}^{N} Y_m = 1$$

$$P = \left(\sum_{m=1}^{N} \frac{Y_m}{M_m}\right) \rho R T$$

$$h_s = \sum_{m=1}^{N} Y_m \, h_{s,m}$$

$$h_{s,m} = \int_{T_{std}}^{T} C_{p,m} dT \quad m = 1 \ldots N$$

$$h_c = \sum_{m=1}^{N} Y_m h_{c,m}$$

$$\tau_{ij} = (\mu + \mu_t)\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k}\right]$$

$$S_{hc} = -\sum_{m=1}^{N} \omega_m h_{c,m}$$

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), S^2 = S_{ij} S_{ij}$$

Here we used the conventional notation. Here ρ is the density, u_j is the velocity, P is the pressure, T is the temperature, h_s is the enthalpy, τ_{ij} is the Reynolds stress tensor, Y_m is the mass fraction for the mth fluid component, K is the specific kinetic energy, ω_m are the species reaction rates, μ , μ_t are molecular and turbulent viscosities, k and ω are kinetic turbulent energy and the dissipation per unit turbulence kinetic energy for k-ω SST turbulence model, S_{ij} is the strain-stress tensor, N is the number of components in mixture.

Boundary conditions

The simulation is run in axisymmetric 2D setting. For modeling in an axisymmetric 2D setting, a sector with a small central angle of 1° is considered. In this case, on the side faces within the OpenFOAM package, one can define boundary conditions of the "wedge" type that do not require specific values, and do not specify boundary conditions on the symmetry axis.

Initial conditions

To simulate the ignition process, following [6], it is assumed that the main chamber and the injectors with fuel and oxidizer adjacent to it are initially filled with nitrogen at a temperature of 1500 *K*. The remaining two-thirds of the length of the injectors are filled with fuel, oxidizer in the proportions specified in the input sections, and also have a temperature of the inlet cross-sections. Such initial conditions provide a relatively "smooth" ignition process without significant oscillations. The Chemkin format of file were used to set up kinetics of the reactions.

Numerical schemes and solvers

The Gauss scalarScheme was used for approximation of convective terms, the Gauss linear scheme was used for approximation of diffusion terms, the Gauss linear corrected scheme was used approximation of laplacian term. To solve linear system equations the PBiCG method with DILU preconditioner was used for pressure, U, h, k, omega values. The tolerance was set to 1e-12. The resulting equations for velocity and pressure coupling were solved by the iterative PIMPLE algorithm with nCorrectors equal to 2.

Computational mesh

For this task, it is required to build a substantially irregular mesh. So in the field of connection of the fuel injector and the main chamber, the injector thickness is of the order of 1 *mm* and the speed is transonic, while in the main chamber with a diameter of about 38 *mm* the velocities are essentially subsonic. On the other hand, near the wall of the main chamber, it is required to provide a sufficiently small cell size in the normal direction to the wall to ensure sufficient accuracy of heat flow calculation. As a tool for constructing a computational grid, the Gmsh mesh generator was chosen, which allows to build 3D grids both with the help of a script in a specialized language and interactively. Figure 3 shows the calculated mesh in the area of the injector and main chamber connection. In the computations, a grid with 26300 cells was used, with the criterion y^+ for the top wall in the main chamber not exceeding the value of 0.6, which is a very good indicator.

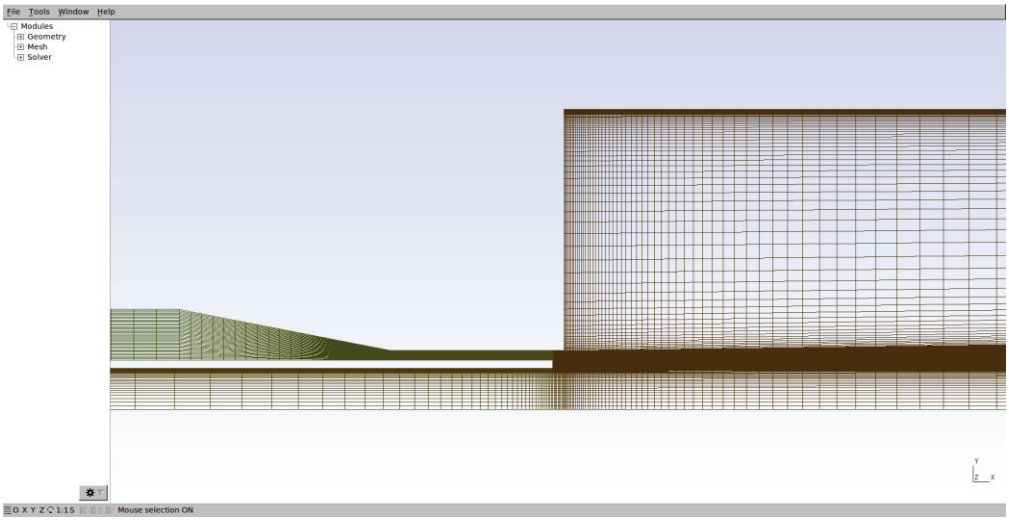

FIGURE 3. Fragment of the computational mesh

Process of computations

The computations were performed on the UniHUB cluster of the ISP RAS using 12-36 cores. The time step was set so that the Courant number did not exceed 0.25. The establishment process required computations in the course of 60 *ms* model time. The continuation of the computation to 100 *ms* did not reveal any changes in the spatial distribution of variables.

RESULTS OF COMPUTATIONS AND DISCUSSION

The value of pressure in the main chamber was 5.22 *MPa* as a result of computations. This value differs less than 0.1% of the measured pressure. The maximum computed temperature is slightly more than 3500 *K* that corresponds to all earlier carried out computations.

The temperature distribution is shown on Fig. 4. The Mass concentration of OH is shown on Fig. 5. It can be seen that the largest gradients are in the vicinity of the coaxial injector between the oxygen and fuel pre burners.

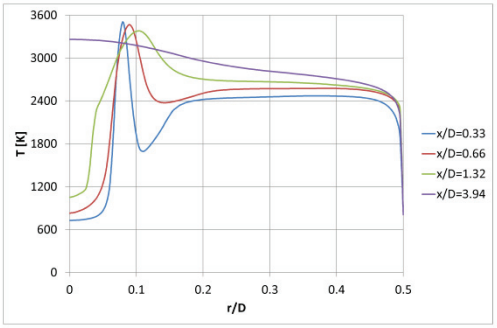

FIGURE 4. Dependence of Temperature from r/D

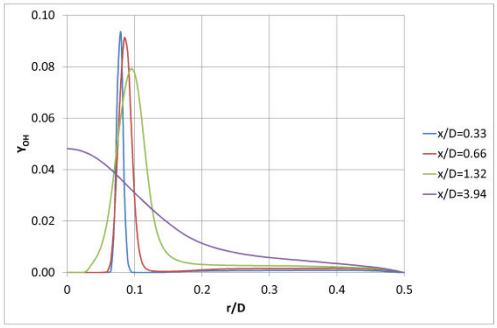

FIGURE 5. Dependence of Mass concentration of OH from r/D

The temperature field distribution is shown in Fig. 6. It can be seen that the region of high temperatures increases with the displacement of nitrogen.

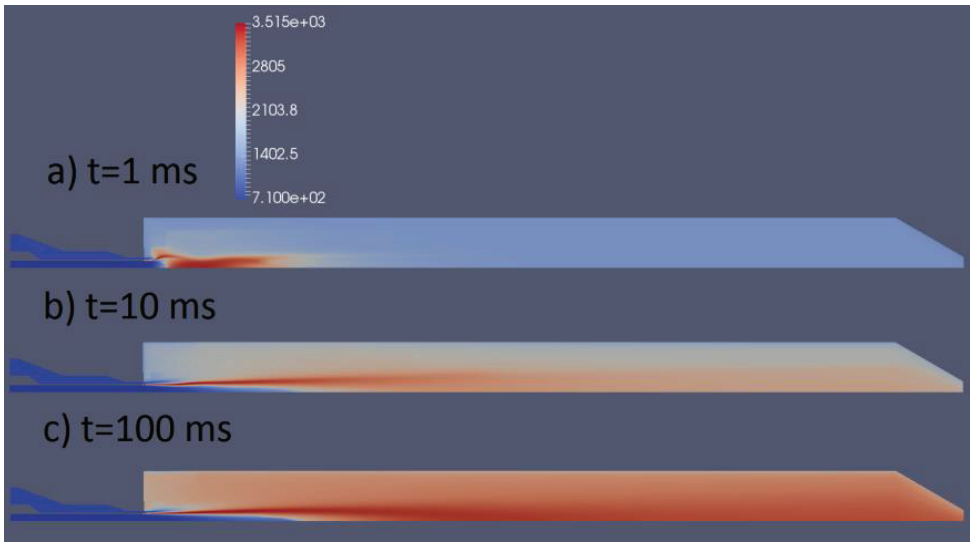

FIGURE 6. The process of ignition. The temperature (K) for a) t=1 ms, b) t=10 ms, c) t=100 ms

Figure 7 shows the steady-state distribution of the absolute value of the velocity. The maximum speed is observed in the narrow part of the fuel injector. A refined mesh is extremely necessary here, since the coarse mesh in this part led to a strong smearing of the fuel velocity and, as a consequence, to a complete cessation of combustion. Computations also show not only the presence of a recirculation zone at the top wall of the main chamber, but also the presence of a small recirculation zone between injectors with fuel and an oxidizer, which is small in size but significant for the formation of combustion.

FIGURE 7. The distribution of the steady-state absolute value of the velocity

Figures 8 and 9 show the steady-state field concentrations of OH and H_2O. Their values agree well with the same distributions from [10-12].

FIGURE 8. The steady-state distribution of the mass concentration of OH

FIGURE 9. The steady-state distribution of the mass concentration of H_2O

CONCLUSION

In the present work, the Penn State test case with combustion chamber has been simulated with the use of the URANS equations. The goal of the simulations has been the measured temperature in the staged hydrogen–oxygen Combustor operating at 750 psia. The current numerical results agree well with the experimental data and the CFD results of other groups [6, 10-12].

Thus, it is possible to draw a conclusion that the solver reactingCentralFoam can be used to simulation of compressible reacting flows.

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