# NUMERICAL SIMULATION OF REACTING FLOWS FOR PROPULSION SYSTEMS

### V.N. Gavriliouk<sup>1</sup>, V. Y. Gidaspov<sup>2</sup>, I. E. Ivanov<sup>2</sup>, A. V. Khokhlov<sup>1</sup>, U. G. Pirumov<sup>2</sup> and V. Y. Streltsov<sup>2</sup>

<sup>1</sup>OOO "NIKA Software", Volokolamskoye sh. 4, Moscow, 125993 Russia <sup>2</sup> Moscow Aviation Institute, Volokolamskoye sh. 4, Moscow, 125993 Russia

The present paper addresses to the questions of simulation of reactive flows in the elements of propulsion engines. Four tasks listed below are considered :

- Numerical modeling of experiments on ignition of reacting mixture in shock tube;
- Flame stabilisation behind a corner flame holder in a premixed benzene-air flow;
- Calculation of the mixing and combusting processes in a liner of air-breathing engine;
- Estimation of thermal loads for the model chamber of oxygen-hydrogen LPRE.

To solve the first task the 2D unsteady Euler system is used [1]. Solution of the other tasks bases on the unsteady Favre averaged 3D Navier-Stockes system with energy and species transport equations and the heat transfer equation for a solid body in combination with the models of thermodynamic properties, phase transition models, models of impulse, energy and mass exchange between liquid and gas phases [2-3].

### 1. Numerical modeling of experiments on ignition of a reacting mixture in the shock tube

Numerical modeling physical experiments in shock tubes on research of diffraction of a shock wave on a rectangular obstacle in reacting gas environment has been made. The shock tube has a cross-section of 38 x 76 mm. The obstacle represents a rectangular block in height equal to a half of the height of the channel and in width equal to the width of the channel. For modeling the chemical transformations of gaseous component the detailed kinetic mechanism describing burning of a hydrogen-oxygen-argon mixture, consisting of 19 reversible reactions and including 10 component was used. The initial pressure was 5.3 KPa, the Mach number on a falling shock wave 2.5. Settlement with great dispatch wave structure of current which consists of a passing shock wave, a reflected shock wave, a front of burning and a front of a detonation wave, which coincides with high accuracy with observable in experiments is obtained.

# 2. Flame stabilisation behind a corner flame holder in a premixed benzene-air flow

Experimental data [4] provide the measured profiles of temperature and turbulence that were used to confirm the numerical model and validity of calculation algorithms for the case of premixed combustion. Experimental rig was the channel of rectangular profile with the corner flame holder located inside. 3D task was solved in this case, because the channel was so narrow that it was impossible to neglect spatial character of a flow and influence of side walls. Additionally, there was a gap between the ends of flame holder and side walls, also accounted in calculation. The simplified reaction mechanism consisting of one conventional reaction was applied. For setting the boundary and initial conditions, the data of turbulence measurements in experiment were used. Inlet benzene-air mixture had the inlet velocity of 150 m/s at 415K and atmospheric pressure. Air excess factor was  $\alpha$ =1.5. Simulation was performed using the unsteady calculation with averaging the temperature field in time. Initially a steady solution was achieved for the cold flow, and then, using it as the initial approach, unsteady calculation was performed until stabilisation. The mixture was "ignited" providing its temporal heating using the local heat source in reverse flow zone. Comparing the experimental and calculated temperature profile on can see a good agreement in size of the reverse flow zone and levels of minimal and maximal temperature. It is possible to conclude that in general the phenomenon was modelled properly.

# 3. Calculation of mixing and combusting processes in a liner of air-breathing engine

Calculation of the chamber of air-breathing engine was performed to estimate the level of heat loads at the liner and the level of pollutants formation at different operating regimes. Geometry of the annular liner used in calculation repeated all geometry features of the developed chamber, including all secondary and minor air supplies used for cooling and maintenance of the combustion efficiency. The boundary conditions for the gas and droplets were set with account of the specifics of gas and droplets supply to the combustion chamber. The flow in the swirler of the main sprayer was calculated simultaneously. In general, the mass flows of air and propellant (kerosene) were set for the chamber. Spectra of the droplet sizes formed in the decay of liquid film, as well as the other start characteristics of polydisperse droplet phase were set using the experimental data. Propagation field of each fraction of droplet phase was calculated using individual Lagrangian mesh formed by the droplet trajectories of certain fraction. Reference trajectories calculated at each time step were started in such a manner that they uniformly and with necessary density passed through the propagation region of each fraction to satisfy the requirements of calculation precision. Initial velocities of droplets were set within some ranges both by direction and magnitude for each starting point. The interaction between fractions was neglected as well as the influence of radiation on the heating of an individual droplet. A numerical mesh had 209542 cells. The commuting time was 62 hours on a personal computer with Athlon XP 1900+. Calculation of pollutants at the exit of the liner provides the basis for optimisation of fuel and air supply from the point of view of pollutions reduction and preservation of the high combustion efficiency. The results achieved in this calculation are in a good agreement with the emission characteristics of similar devices [5].

### 4. Estimation of thermal loads for the model chamber of oxygen-hydrogen LPRE

For optimising the working process in the chamber of LPRE, it is necessary to take into account such factors as temperature impact on the walls, combustion efficiency, losses related to the friction and deviation from equilibrium, losses related to the imperfect geometry. To illustrate the potentials of the proposed models calculation of heat loads on the walls of the combustion chamber was performed. The specific features of the problem were that the cryogenic propellant components were supplied to the chamber, and one of the components (oxygen) was liquid at supercritical conditions. The reactions of components had a non-equilibrium character, and the process of mixing and combustion had a significantly unsteady character. It was also necessary to calculate the boundary layer flow and derive the heat exchange factor. To approximate the properties of supercritical oxygen the special state equation was used. Chemical reactions in the gas were described using the mechanism of 19 reversible stages for eight components. The object of simulation was the experimental subscale caloric chamber [6]. The chamber was divided across into segments and for each segment the amount of heat was measured. Unsteady approach is convenient, where it is necessary to take into account the unsteady character of the flow, and it provides the straightforward and simple agreement of gas-dynamic and chemical time scales together with a possibility to simulate the ignition process. To achieve averaged values the instant temperature and heat flows were accumulated within some period of time. The calculation was finished after stabilisation of averaged parameters. To accelerate the calculation the procedure of splitting of physical processes was used in combination with SMP model of parallel computing of chemical kinetics equations.

#### **5.** Conclusions

The proposed method of calculation of the reacting biphasic mixtures is in satisfactory agreement with the experimental data and can be used for development and optimisation of different purpose combustion chambers. The method provides local, integral and emission characteristics of combustion chambers.

#### Acknowledgements

The research described was partially supported by the Russian Fund of Fundamental Research (grants N 03-01-00866-a and 04-01-81012-BEL2004 a).

#### References

- [1] Gidaspov V.Yu., Ivanov I.A., Kryukov I.A. Numerical modelling of initiation of a detonation in the focusing channel // Mathematical modeling. V. 4. N 12, 1992. P. 85-88.
- [2] Volkov V.A., Musin V.R., Pirumov U.G., Prokhorov M.B. and Strel'tsov V.Yu. Numerical modelling of carbon monoxide neutralization by metered water injection into a high-temperature mixture of combustion products //Izv.Rossiiskoi Akad. Nauk,Mekh. Zhidk. Gaza.1993.N 6.P. 96-106.
- [3] Thomas G.O., Ward S.M., Williams R.Li., Bambrey R.J. On critical conditions for detonation initiation by shock reflection from obstacles // Shock Waves, 2002, №12, pp. 111-119.

- [4] Solntsev V.P., Golubev V.A. Research of process of combustion of a benzene-air mixture in conditions of interaction of the turbulent track formed by stabilizers / News of higher educational institutions MHE the USSR, a series "Aviation technics ", 1959
- [5] Lister D. ICAO Engine Exhaust Emission Data Bank, update 2003, based on ICAO doc 9646, 1995.
- [6] Preclic D et.al. Cryogenic Rocket Calorimeter Chamber Experiments and Heat Transfer Simulations. //AIAA 98-3440.