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NUMERICAL INVESTIGATION OF COMBUSTION EQUILIBRIUM IN THRUST CHAMBERS OF
LIQUID ROCKET ENGINES

Abstract

Determination of the chemical equilibrium composition of the combustion products is a topic of major interest in the preliminary design of Liquid Rocket Engines (LRE). A significant quantity of various methodologies used to conduct the chemical equilibrium composition has been developed until now. However, an accurate study of these methodologies reveals the fact that various mathematical models have been developed for various computational conditions (combustion chamber temperature, mixture ratio, etc.). At the same time, various approaches and methods to conduct the chemical equilibrium analysis for various propellant configurations were proposed by various researchers. However, these methods do not operate effectively for the oxidizer excess coefficient $0.01 \leq \alpha \leq 0.1$ ($T_c \leq 1500$ K, $p_c > 50$ MPa). Therefore, a generalized tensor model which would be unique such that it would be capable of being applied for any case by, hence, yielding correct results is still absent.

In the existing studies the chemical equilibrium analysis problems listed below have not been solved due to their uncertainties:

- final composition of combustion products;
- possibility of existence of an equilibrium state described by this mathematical model under any considered conditions in a wide range of the oxidizer excess coefficient and combustion temperature values;
- completeness, non-redundancy and non-inconsistency of used thermochemical models for equilibrium state;
- convergence of the numerical solution of equilibrium state models for any physical calculation conditions;
- adequacy of the numerical calculation results to the known physical-chemical principles.

The solution of these problems requires a large number of numerical experiments and evidential comparison of the results of numerical calculations with experimental data.

Development of a model for the analysis of the equilibrium state and its numerical implementation for a large range of the oxidizer excess coefficient and combustion temperature values does not allow the efficient use of computer resources due to the high array dimensions and large differences among the elements of these arrays. Therefore, it is necessary to apply the tensor mathematics for the thermodynamic calculation of the parameters of multicomponent reactants' mixtures in the thrust chamber of LRE. Considering the information presented above, a tensor model for the chemical equilibrium analysis of the combustion process is considered in this paper. Considered an example combustion problem, in which as the fuel and oxidizer components liquid methane CH₄ and liquid oxygen O₂ are presented, respectively. It has been proved, that the tensor model of the equilibrium behaves stably meaning that the solution does not diverge.