

The equations of state of methane, oxygen, and their mixtures: Calculation of the temperature and pressure of the mixture in the combustion chamber of liquid rocket engine before ignition

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At present, the leading space nations pay great attention to the development of liquid rocket engines (LRE) on environmentally clean fuel components – oxygen and liquefied natural gas – for reusable-flight launch vehicles. In the design of the combustion chambers of LREs there is a question about the characteristics of the fuel components and their mixtures in the vicinity of the bottom of the injector head. The purpose of this work is the development of methods for calculating the thermodynamic parameters of oxygen–methane mixture in the combustion chamber prior to ignition, i.e. in the course of fuel components injection into the combustion chamber and their subsequent mixing.

In [1, 2] on the basis of the available data in the literature and our own calculations, we obtained the thermal and caloric equation of state (EOS) of methane and oxygen in an analytical form. The thermal EOS of methane gas [1] provides a good accuracy of the calculation of P– ρ –T data in the pressure range 0.1 MPa <P <100 MPa and supercritical temperature range of 250 K <T <1000 K. The error in pressure is on average less than 1% and the maximum error attributable to a relatively small region of temperature and density is 4.2%. Similar EOS for oxygen [2] provides the same calculation accuracy of P– ρ –T data in a wide range of pressures and temperatures. The caloric EOS for methane and oxygen were derived using the reference data of the spectroscopic frequencies (characteristic temperatures of intramolecular vibrations for methane ($\Theta_1(1) = 4197$ K, $\Theta_2(2) = 2206$ K, $\Theta_3(3) = 4344$ K, $\Theta_4(3) = 1886$ K) and for oxygen ($\Theta = 2273$ K)).

Based on these EOS, we resolved several problems that demonstrate the method for calculating the thermodynamic parameters of oxygen–methane mixture in the combustion chamber prior to ignition:

- calculated the temperature and pressure of the equilibrium state of the mixture after feeding and mixing of the components and the establishment of equilibrium temperature;
- examined several known mixing rules and proposed the EOS for a mixture of real gases;
- calculated the density of the mixture for given values of the common pressure and temperatures of the components, and
- calculated the density of the mixture for given values of the common pressure and equilibrium temperature of the mixture in the combustion chamber.

As an example, we present calculations for the conditions when a LRE combustion chamber is fed with oxygen at $T_2 = 110$ K and methane at $T_1 = 850$ K at the oxidizer-to-fuel mass ratio in the engine equal to 3.4. Note that isotherm $T_2 = 110$ K is below the critical temperature of oxygen, so it passes through the single-phase regions of vapor and liquid and through the two-phase liquid–vapor region.

References

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2. Kuznetsov N.M., Dubrovsky A.V., Frolov S.M. Analytical approximation of the thermal and caloric equations of state for real gases over a wide density and temperature range. Russian Journal of Physical Chemistry B, 2011, Vol. 5, No. 7, pp. 1084–1105.