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MEANS FOR GRAPHIC INTERPOLATION OF THE RESULTS OF CALCULATIONS OF CHEMICAL NONEQUILIBRIUM FLOWS IN NOZZLES

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ABSTRACT: On the basis of an analysis of the function which describes the rate of heat release in the process of the recombination of high temperature, dissociated combustion products in a supersonic nozzle, we will show that the degree of approximation of the value of the gas flow impulse upon the exit from the nozzle to its equilibrium value with fixed elementary composition and total enthalpy of the gas is proportional to the square of the pressure upon entrance to the nozzle p_k^2 and to the characteristic linear dimension of the nozzle L. On this basis we propose a method for graphic interpolation of the results of calculations, presented in the form of a relationship between the impulse loss of the flow and the product Lp_k^2.

With the expansion of a high temperature mixture of dissociated gases in a supersonic nozzle a recombination process takes place accompanied by the transfer of dissociation energy into the thermal energy of the flow. When the gas remains in the nozzle long enough to complete the recombination reaction, the flow will be near to an equilibrium system. In the opposite case, the parameters of the flow deviate from equilibrium and impulse losses of the gas stream ΔI arise caused by the incomplete transfer of the chemical energy of the gas to thermal energy. /284

A calculated estimate of these losses for complex gas mixtures such as combustion products even in a one-dimensional framework, presents a time-consuming problem, due to the large amount of machine time required on a computer [1]. Therefore, it would be desirable to represent the results of calculations, obtained for any concrete parameters of the flow in the nozzle, in a form which would allow us to convert them easily to apply to their flow conditions.

It follows from an analysis of calculated investigations of nonequilibrium flows in nozzles, that the degree of approximation of the flow parameters to their equilibrium values is determined by the intensity of the heat release in the process of recombination, which in turn is proportional to the velocity of elementary tri-

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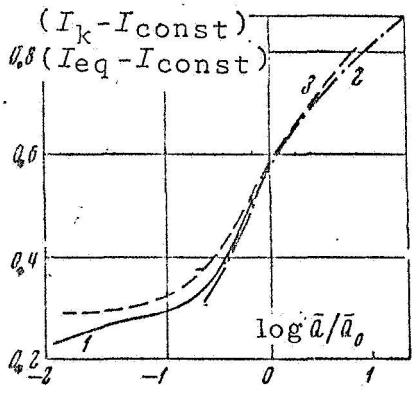
* Numbers in the margin indicate pagination in the foreign text.

molecular reactions such as $H + H + M \rightarrow H_2 + M$, and also to the time the gas is present in the nozzle [2]. The equation describing the heat release along the nozzle has the following form:

$$\bar{Q} = \frac{dQ}{d\varepsilon} = \sum_{i=1} Q_i \frac{dq_i}{d\varepsilon} = \frac{L}{v}\frac{dx}{d\varepsilon}\rho^2 \sum_{i=1} Q_i k_i f(T, q_j), \qquad (1)$$

where Q_i is the thermal effect of the i-th trimolecular reaction; ε is the area of the cross section of the nozzle, relative to the area of the critical cross section; q_i is the mass concentratation of matter formed in the i-th reaction; L is the characteristic linear dimension, for example the radius of the ordinate of the neck of the nozzle; ρ is the density of the gas; x is a dimensionless coordinate relative to L; v is the velocity of the gas; k_i is the reaction rate of the i-th reaction; n is the number of trimolecular reactions, resulting in the mixture; $j = 1,\ldots,N$ where N is the index of the component of the gas mixture /28

In certain simple cases the expression for the value of $dx/d\varepsilon$, which characterizes the shape of the nozzle, can be obtained analytically. Thus for a plane wedgeshaped nozzle with an angular point $dx/d\varepsilon = 1/\tan 1/2\theta$ (where $1/2\theta$ is the half-angle of the opening of the nozzle).



The Influence of the Intensity of Heat Release $\bar{Q}$ on the Impulse Loss of the Gas Flow on the Nozzle: H_2+F_2; $\alpha = 0.42$; $\varepsilon = 40$. At the Initial Point with $\log(\bar{Q}/\bar{Q}_0) = 0$; $p_k = 21$ atm; $R = 1.5\ t$; $J_p = 475$ sec; $J_d = 434.5$ sec (1) $p_k = 4.2$ atm, L = var; (2) $p_k = 21$ atm; L = var; (3) $p_k = 21$ atm, $R = 1.5\ t$; k_1 = var.

In equation (1) the product $Ldx/vd\varepsilon$ determines the time the gas is present in a unit section of the nozzle, and the remaining factors in the right-hand side determine the heat release rate in the process of recombination.

An examination of the numerical values included in the right-hand side of equation (1) indicates the following. If in the case of a flow of a gas mixture such as dissociated combustion products across a nozzle the total enthalpy of the gas in front of the nozzle and the mass relationship of the elements in the mixture are fixed (with a given excess oxidant ratio α) and the pressure at the entrance to the nozzle or the dimension and shape of the nozzle vary, then in an arbitrarily chosen cross section of the nozzle (cf, for example, [3]) the product $L\rho^2$ will vary the most (up to an order of magnitude) when the values of v, T and q vary relatively little. The value of $d\varepsilon/dx$ for nozzles similar in shape can also be assumed to be constant with an

accuracy of a few tenths of a percent.

Considering that in these circumstances with variation of the pressure in front of the nozzle, the variations in gas temperature in the nozzle are rather small, we can assume also that the gas density ρ in a given cross section of the nozzle is proportional to the pressure on entrance to the nozzle (pressure in the combustion chamber). Thus, in this case the intensity of the heat release in the process of recombination and, consequently, the impulse loss of the flow are mainly determined by the product Lp_k^2. This allows us to present the results of the calculations of nonequilibrium flows in a form which is convenient for practical use, treating the data as a function of the term Lp_k^2.

As an example of a flow of the products of hydrogen-fluorine combustion in a nozzle, the figure shows that the data obtained for a constant oxidant excess ratio with various values of the pressure at the entrance to the nozzle p_k and absolute dimensions of the nozzle L, with similar interpretation actually lie practically on the same curve. In this case we used the results of calculation obtained in reference [2] for a geometric expansion level $\varepsilon = 40$; $\alpha = 0.42$; $p_k = 4.2$ atm (Curve 1) and 21 atm (Curve 2) with the thrust of the nozzle changing within the range $R = 0.045 - 45\ t$. In the figure, along the abscissa we plotted the change in the value of

$$\overline{Q} / \overline{Q}_0 = Lp_k^2 / (Lp_k^2)_0, \tag{2}$$

where $\overline{Q}_0$ is the value of $\overline{Q}$, corresponding to the initial, arbitrarily chosen conditions of the flow in the nozzle, namely $p_k = 21$ atm and $R = 1.5\ t$. In interpreting the data we took into consideration that the thrust of the nozzle is proportional to the area of its critical cross section, which for axisymmetrical nozzles, discussed in reference [2], in turn, is proportional to the square of the characteristic dimension of the nozzle L^2. Along the ordinate we plotted the dimensionless value $(I_k - I_{const})/(I_{eq} - I_{const})$, characterizing the amount of dissociation energy returned to the flow /28 in the process of recombination. Here I is the flow impulse and the indices k, eq and const refer respectively to the calculations of equilibrium gas, taking into account chemical kinetics and with a constant composition of the gas along the nozzle[1]. It follows from the figure that Curves 1 and 2 practically coincide. Their divergence at the value 0.02 - 0.03 for $(I_k - I_{const})/(I_{eq} - I_{const})$ is insignificant since, according to the estimating calculations, made on the basis of the data of reference [2], they correspond to a deviation in the value of I_k of less than 0.3%.

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[1] We can use the value $(I_{eq} - I_k)/I_{const}$ as a parameter characterizing the impulse loss of the gas flow in the nozzle with the same success.

The proposed method is in principle valid only for comparatively large values of the level of expansion of the nozzle ε, when the flow parameters have a definite deviation from the equilibrium values. With transfer to small values of ε the situation may arise when with a large value p_k of the comparable pressures, expansion up to this cross section is equilibrium: $(I_k - I_{const})/(I_{eq} - I_{const}) \approx 1$, and with a small value of p_k the flow is already nonequilibrium: $(I_k - I_{const})/(I_{eq} - I_{const}) < 1$. With the approach to these conditions, the curves, analogous to those shown in the figure, will not coincide. However, in this case, as a rule, $(I_{eq} - I_{const}) \ll I_{eq}$ and the noticable divergence in the curves will not have any practical significance. Therefore, we can substantiate that the generality of the results illustrated by curves 1 and 2 in essence is not limited by the choice of the value of ε.

The obtained function is naturally not universal, and depends on the initial elementary composition of the gas mixture, and also its total enthalpy, and can be used only for interpolation of the results of calculations with a given ε and variation in p_k or L.

The examined graph in certain circumstances can be used also for an evaluation of the precision of the results of calculations. We know that the values of the constants of elementary trimolecular reaction velocities, which determine the development of the recombination process, at high temperatures ($T \geq 1000°K$) are, at the present time, as a rule, known only with an accuracy of about an order of magnitude [4]. In connection with this, the difference in the constant values we used rarely leads to a noticeable divergence in the results of the calculations. Therefore, when using the data of the various references, it may be necessary to take into account the influence of the disagreement of the constant values used in the calculations.

When the process of recombination in the nozzle is limited by the occurance of only one trimolecular reaction (and, consequently, the accuracy of the calculation is determined basically by the choice of the value of its reaction velocity), the introduction of such a correction presents no great difficulties, since in this case a change in the value of k_i is mathematically equivalent to a change in L (cf. equation (1)). In solving a similar problem, this allows us to use the graphic interpretation of the results of the calculations which we described earlier. In this case in the parameter $\overline{Q}$ which accounts for the intensity of the heat release in the nozzle, as a variable we should take into account the value of the velocity constant which limits the process of trimolecular reaction k_i

$$\overline{Q} / Q_0 = k_i L p_k^2 / (k_i L p_k^2)_0. \qquad (3)$$

It is obvious that if k_i = idem, then expression (3) is automatically reduced to (2). The validity of these arguments is substantiated

by the results of a calculated estimate of the influence of the choice of the values for the recombination velocity constant for atomic hydrogen, as shown in the figure. Reference [2] showed that with a flow of combustion products $H_2 + F_2$ in a nozzle with α = 0.42 (the conditions examined in the figure) the choice of reaction velocity $H + H + M \xrightarrow{k_1} H_2 + M$ has a strong influence on the value for the impulse of the flow obtained in the calculation and the corresponding quantitative data are introduced. Conversion of these data according to equation (3) is shown in the figure as curve 3. We can see that it practically coincides with curves 1 and 2 which characterize the influence of the values of L and p_k on the value of the flow impulse. /28

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