N. A. ANFIMOV

1964

SovietRxiv

Abstract

Full Text

HYDROMECHANICS

N. A. ANFIMOV

DIFFUSIONAL SEPARATION OF A GAS MIXTURE IN THE PRESENCE OF DISSOCIATION

(Presented by Academician G. I. Petrov on 16 January 1964)

In paper (^{1}) an effect of diffusional separation of a gas mixture in the presence of dissociation was described. This effect consists in the fact that, when there is a temperature difference in a boundary layer consisting of a mixture of dissociating gases, the elemental composition of the gas at the surface differs from the composition of the external flow. Separation of the mixture is caused by differences in the diffusion coefficients of the individual components. The present work is devoted to studying the influence of various factors on the effect of diffusional separation of the boundary layer.

The simplest three-component gas mixture is considered, consisting of the products of dissociation of a diatomic gas A_2 and a neutral (inert) gas B. The phenomenon of separation of the boundary layer is investigated for the neighborhood of the critical point of an axisymmetric blunt body. The following assumptions are made:
a) the rate of the chemical reaction

$$A_2 \rightleftarrows 2A$$

is equal to zero in the boundary layer and infinitely large at the surface of the body;
b) thermal diffusion inside the boundary layer is absent.

The system of equations of the multicomponent boundary layer and the boundary conditions for the case under consideration are given in paper (^{1}). The method of numerical integration of the resulting system of equations is also described there, as well as a method for calculating the thermodynamic and transport properties of gas mixtures. We shall only note that, in calculating the transport properties of the individual components, it was assumed that the laws of interaction of all atoms and molecules are determined by the Lennard-Jones potential.

In the present work the results are given of numerous calculations carried out for various gas mixtures at diverse values of the parameters in the external flow and at the wall. The following gas mixtures were considered: O—O_2—N_2; O—O_2—He; O—O_2—Kr; H—H_2—He; H—H_2—N_2; H—H_2—Kr; J—J_2—Kr. The temperature and pressure in the incident flow were varied within such limits that the degree of dissociation of gas A_2 changed from 0 to 1. In the present work, by the degree of dissociation is meant the mass content of atoms in the dissociation products of the gas

$$\alpha = \frac{C_A}{C_A + C_{A_2}}.$$

The concentration of the neutral gas B in the incident flow was varied from 0 to 1. The temperature of the body surface was assumed to be so low that complete recombination of the gas A_2 occurred there.

In the main part of the calculations it was assumed that the surface of the body is impermeable, i.e., the gas flow through this surface is equal to zero. However, calculations were also carried out for the case when uniform suction of gas from the boundary layer occurs through the surface, as well as injection of a foreign gas into the boundary layer.

The phenomena leading to diffusional separation of the boundary layer have a simple qualitative explanation. The flux of atoms A is directed from the hotter region into the colder one. If the temperature of the flux is higher than the surface temperature, then the flux of atoms is directed toward the wall, while the flux of molecules A_2 has the opposite direction. Because of the difference in diffusion coefficients, atoms A penetrate to the wall more easily than molecules A_2 penetrate in the opposite direction, as a result of which, near the surface, the content of gas A_2 increases in comparison with the external flow.

As a result of numerous calculations it was established that the magnitude of diffusional separation at an impermeable surface is determined by the following factors: (a) the degree of dissociation of gas A_2 in the external flow; (b) the concentration of gas B in the external flow; (c) the ratio of the diffusion properties of the atoms and molecules of gas A_2.

In this case the expression for diffusional separation can be represented in the form

$$\Delta = C_{B_e} - C_{B_w} = f_1(\alpha) f_2(C_{B_e}) f_3 \left(\frac{\sigma_{A_2}^2 \Omega_{A_2}^{(1,1)}}{\sigma_A^2 \Omega_A^{(1,1)}} \right), \tag{1}$$

where C_i is the mass concentration; σ_i is the effective cross section; $\Omega_i^{(1,1)}$ is the collision integral. The subscript w denotes values of the parameters at the wall, and e at the outer boundary of the boundary layer.

The results of numerical calculations show that the functions f_1, f_2, and f_3 are universal in character. For these functions the following approximate expressions were proposed:

$$f_1(\alpha) = 1.2\alpha - 0.2\alpha^2; \tag{2}$$

$$f_2(C_{B_e}) = 1.97C_{B_e}(1 - C_{B_e})(1.5 + C_{B_e}); \tag{3}$$

$$f_3\left(\frac{\sigma^2_{A_2}\Omega^{(1,1)}_{A_2}}{\sigma^2_{A}\Omega^{(1,1)}_{A}}\right) = 0.08\left(\frac{\sigma^2_{A_2}\Omega^{(1,1)}_{A_2}}{\sigma^2_{A}\Omega^{(1,1)}_{A}} - 1\right)^{0.6}. \tag{4}$$

The maximum error of the approximation is 1% for the function f_1, 4% for the function f_2, and 6% for the function f_3.

In order to prove the independence of the separation effect from the remaining parameters, special calculations were carried out. For example, the pressure and temperature of the incident flow were varied in such a way that the degree of dissociation of gas A_2 remained constant. When oxygen was considered as the dissociating gas, the following pairs of values of the indicated parameters were used: (a) $p = 10$ atm., $T = 6000$°K; (b) $p = 1.26$ atm., $T = 5000$°K; (c) $p = 0.0571$ atm., $T = 4000$°K.

Despite the considerable change in temperature and pressure, the separation effect of mixtures of oxygen with various neutral gases remained constant to within 0.4%. The properties of gas B also have only a weak influence on the magnitude of the separation.

Dissociated air, generally speaking, does not always fit within the framework of the simplified scheme A—A_2—B investigated in the present work. Formal calculations by formulas (1)–(4) give satisfactory results only in that range of temperatures and pressures where the dissociation of oxygen is already significant, while nitrogen is practically not yet dissociated. This fact was already noted in work (^{1}).

After the onset of nitrogen dissociation, the separation effect of air should decrease, because the analogous effect for dissociated nitrogen neutralizes the increase in the oxygen content at the surface. One may attempt to determine the separation effect for real dissociated air by means of formulas (1)–(4), calculating the function $f_1(\alpha)$ at a certain effective value of the degree of dissociation

$$\alpha^* = \alpha_O - \alpha_N, \tag{5}$$

where

Fig. 1

Figure 1: Fig. 1

Fig. 2

Figure 2: Fig. 2

$$\alpha_O = \frac{C_{O_e}}{\left(C_O + C_{O_2} + {}^{16}/_{30} C_{NO}\right)_e} = \frac{C_{O_e}}{0.2314},$$

$$\alpha_N = \frac{C_{N_e}}{\left(C_N + C_{N_2} + {}^{14}/_{30} C_{NO}\right)_e} = \frac{C_{N_e}}{0.7686}.$$

In Fig. 1 the approximate calculations of air separation by formulas (1)–(5) are compared with the exact solution described in [2]. It can be seen that the approximate calculations qualitatively correctly reflect the separation effect; however, in some cases the quantitative discrepancies prove to be considerable. In addition, the approximate formula does not make it possible to detect the change in sign of the effect of diffusional separation of air at high temperatures, when the degree of dissociation of nitrogen is close to unity.

Fig. 1. Dependence of the oxygen concentration on the cold impermeable surface in air on the stagnation temperature.
a –exact solution [2], *b* –formulas (1)–(5); 1 –$p = 0.1$ atm., 2 –$p = 10$ atm.

Fig. 2. Dependence of the relative magnitude of the separation effect on the value of the flow function at the wall when gas is withdrawn through the surface.
1 –O–O_2–N_2, 2 –H–H_2–He

In an analogous manner one can introduce a correction in the case when the degree of dissociation of the gas at the surface differs from zero. In this case the difference between the values of the degree of dissociation at the outer boundary of the boundary layer and at the wall should be substituted into formula (2).

In connection with the practical use of the effect of diffusional separation of a gas mixture in the presence of dissociation, the question arises of the influence of gas withdrawal from the boundary layer through the surface on the magnitude of this effect. The corresponding calculations showed that withdrawal of gas from the boundary layer leads to a reduction of the separation effect. This result is illustrated in Fig. 2, where the dependences of separation for the mixtures O –O_2–N_2 and H–H_2–He on the flow function at the wall, proportional to the gas flow rate through the surface, are shown. It can be seen that, at small flow rates, the decrease in separation of gas mixtures is a linear function of the flow rate, weakly dependent on the composition of the boundary layer.

If withdrawal of gas from the boundary layer leads to a weakening of the separation effect, then blowing a foreign gas through the surface strengthens this effect.

Calculations carried out for bodies of another shape (a plane critical point, a plate) showed that the magnitude of the effect of diffusional separation changes in this case by no more than 1–2%.

Naturally, the effect of diffusional separation of a gas mixture in the presence of dissociation can be used for separating mixtures of dissociating gases or the dissociation products of some complex gas.

Moreover, establishing a dependence of type (4) makes it possible to use the effect of diffusion separation for the experimental determination of the diffusion properties of certain gases (O_2, N_2, H_2, etc.) in the atomic state. At present there are no reliable methods for measuring these properties. Expression (1) directly relates the diffusion properties of atoms to the magnitude of the separation effect. In this connection, the diffusion properties of molecules may be regarded as known.

The main limitation here is the still unclear character of the influence of the finite rate of chemical reactions within the boundary layer on the magnitude of the separation effect. The present calculations have been carried out for a frozen boundary layer; analogous calculations should be carried out for an equilibrium boundary layer, and also for the case of a finite rate of chemical reactions in the gas phase.

Received
15 I 1964

REFERENCES

1. N. A. Anfimov, *Izv. AN SSSR, Mekh. i mashinostr.*, No. 5, 117 (1963).
2. N. A. Anfimov, *Prikl. mekh. i tekhn. fiz.*, No. 1 (1964).

Note: Figure translations are in progress. See original paper for figures.

Source: Math-Net.Ru and CyberLeninka. Machine translation. Verify with the original.