HEAT AND MASS TRANSFER DURING THE LAMINAR FLOW OF DISSOCIATING N_2O_4 GAS IN A TRIANGULAR BUNDLE OF CYLINDERS

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The problem of heat and mass transfer during the laminar flow of a dissociating gas in a triangular bundle of rods is analyzed. The solution is obtained by numerical means.

In the study of a whole series of modes of operation of various heat-exchange devices it is desirable to have the fullest information on heat exchange in the rather common configuration which consists of a bundle of longitudinally bathed cylinders. This mode of flow with the condition of thermal stabilization has been examined rather thoroughly in the case of the flow of liquid metals [5-7] and of chemically inert substances [2]. However, the effects of heat and mass transfer during the flow of dissociating gases, almost unstudied at present, are of particular interest in connection with the prospects of their use as the coolants for fast-neutron nuclear power plants [1].

In the case when N chemical reactions, in which k components take part, occur in a volume the equations of conservation of energy and mass have the form

$$\rho \frac{DH}{d\tau} = \operatorname{div}\left(\lambda_f \operatorname{grad} T - \sum_{k=1}^{K} h_k j_k\right), \tag{1}$$

$$\rho \frac{DC_k}{d\tau} = -\operatorname{div} j_k + J_k, \tag{2}$$

where

$$H = \sum_{k=1}^{K} h_k C_k. \tag{3}$$

After the substitution of (3) and (2) into (1) the energy equation takes the form

$$\sum_{k=1}^{K} \rho C_k \frac{Dh_k}{d\tau} = \operatorname{div}(\lambda_f \operatorname{grad} T) - \sum_{k=1}^{K} \operatorname{div}(h_k j_k) + \sum_{k=1}^{K} h_k \operatorname{div} j_k - \sum_{k=1}^{K} h_k J_k. \tag{4}$$

Since

$$\frac{Dh_k}{d\tau} = c_{pfk} \frac{DT}{d\tau},$$

$$\sum_{k=1}^{K} \operatorname{div}(h_k j_k) = \sum_{k=1}^{K} h_k \operatorname{div} j_k + \sum_{k=1}^{K} j_k \operatorname{grad} h_k,$$

and, according to the Hess law,

$$\sum_{k=1}^{K} h_k J_k = \sum_{l=1}^{K} Q_{pl} I_l,$$

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the energy Eq. (4) can be written in the following form:

$$\rho c_{pf}\frac{DT}{d\tau}=\operatorname{div}(\lambda_f \operatorname{grad} T)-\sum_{l=1}^{N} Q_{pl}I_l-\sum_{k=1}^{K} j_k c_{pfk}\operatorname{grad} T, \tag{5}$$

where

$$c_{pf}=\sum_{k=1}^{K} c_{pfk}C_k. \tag{6}$$

Now suppose the reaction of dissociation of nitrogen tetroxide occurs in the stream:

$$N_2O_4 \rightleftarrows 2NO_2 \rightleftarrows 2NO + O_2.$$

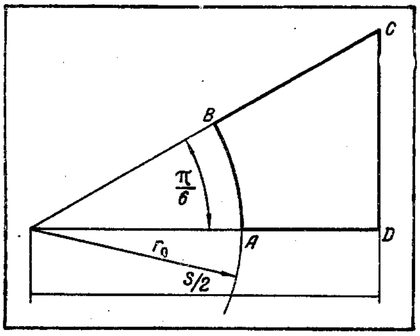

Fig. 1. Elementary cell of the channel.

We assume that the stoichiometric relations are satisfied in the stream, the flow is hydrodynamically stabilized, the "frozen" thermophysical properties do not depend on the temperature and pressure, and the heat capacities of the individual components of the mixture are approximately equal to one another. The latter approximation allows one to neglect the term $\sum_{k=1}^{K} j_k c_{pjk}\operatorname{grad} T$. In addition, because of the symmetry of the infinite system of smooth cylinders, arranged in staggered order, one can analyze the region ABCD shown in Fig. 1. In this case the system of differential equations of heat and mass transfer takes the form

$$\omega\frac{\partial\theta}{\partial\xi}=\frac{\delta^2}{R}\cdot\frac{\partial}{\partial R}\left(R\frac{\partial\theta}{\partial R}\right)+\frac{\delta^2}{R^2}\cdot\frac{\partial^2\theta}{\partial\varphi^2}-\bar{Q}_{p1}\mathrm{Da}_1\mathrm{Le}_1-\bar{Q}_{p2}\mathrm{Da}_4\mathrm{Le}_4, \tag{7}$$

$$\frac{\omega}{\mathrm{Le}_1}\cdot\frac{\partial C_1^*}{\partial\xi}=\frac{\delta^2}{R}\cdot\frac{\partial}{\partial R}\left(R\frac{\partial C_1^*}{\partial R}\right)+\frac{\delta^2}{R^2}\cdot\frac{\partial^2 C_1^*}{\partial\varphi^2}+\mathrm{Da}_1, \tag{8}$$

$$\frac{\omega}{\mathrm{Le}_4}\cdot\frac{\partial C_4^*}{\partial\xi}=\frac{\delta^2}{R}\cdot\frac{\partial}{\partial R}\left(R\frac{\partial C_4^*}{\partial R}\right)+\frac{\delta^2}{R^2}\cdot\frac{\partial^2 C_4^*}{\partial\varphi^2}+\mathrm{Da}_4. \tag{9}$$

The composition of the remaining components of the system is found with the help of the stoichiometric equations.

The field of velocity ω for the stabilized isothermal flow was determined by Sparrow and Loeffler [2] and is found from the equation

$$\omega=\frac{U_x}{\bar{U}}=\frac{1}{2}\beta\,\mathrm{Re}\left(\frac{t}{\delta}\right)^2\left\{\frac{\sqrt{3}}{\pi}\ln R-\frac{1}{4t^2}(R^2-1)+\sum_{i=1}^{p}\frac{\delta_i^*}{6i}\left(\frac{R}{t}\right)^{6i}\left(1-\frac{1}{R^{12i}}\right)\cos 6i\varphi\right\}, \tag{10}$$

where

$$\beta\,\mathrm{Re}=\frac{4\varkappa}{1-\varkappa}F(t), \tag{11}$$

$$\varkappa=1-\frac{\pi/6}{t^2\operatorname{tg}\frac{\pi}{6}}. \tag{12}$$

The values of the coefficients δ_i^* and the function F(t) are presented in [2] and [3], respectively.

The solution of the system of differential Eqs. (7)-(9) is rather complicated. In the case of heating, however, the dissociation of N_2O_4 takes place almost sequentially in two stages. The first stage proceeds rather rapidly and can be taken as an equilibrium stage [1]. The separate study of the heat exchange of the first and second stages of dissociation is therefore justified to a certain extent, with Eqs. (7), (8) ($\mathrm{Da}_4 \equiv 0$, $C_4 \equiv 0$) being considered first and then Eqs. (7), (9) ($\mathrm{Da}_1 = 0$, $C_1^* = 0$).

The solution of the problem of heat exchange with boundary conditions of the second kind in the case of the occurrence of only the first equilibrium stage of N_2O_4 dissociation in the channel can be simplified considerably in the case of Le = 1, since one can then obtain an equation for the dimensionless enthalpy which coincides with the energy equation for the flow of a chemically inert gas. For this it is enough to multiply Eq. (8) by $\bar{Q}_{p1}$ and add it to Eq. (7) with $\mathrm{Da}_4 \equiv 0$. Finally, we have

TABLE 1. Results of Calculation Based on Eqs. (27) and (29)

ξ	$t=1{,}05$		ξ	$t=1{,}1$		ξ	$t=1{,}3$	
	$\bar{\theta}_f$ (29)	$\bar{\theta}_f$ (27)		$\bar{\theta}_f$ (29)	$\bar{\theta}_f$ (27)		$\bar{\theta}_f$ (29)	$\bar{\theta}_f$ (27)
$0{,}7\cdot10^{-3}$	$1{,}208\cdot10^{-3}$	$1{,}208\cdot10^{-3}$	$0{,}7\cdot10^{-3}$	$1{,}87208\cdot10^{-3}$	$1{,}858\cdot10^{-3}$	$0{,}2\cdot10^{-1}$	0,013816	0,013768
$0{,}4\cdot10^{-2}$	0,006904	0,006884	$0{,}4\cdot10^{-2}$	0,010639	0,010639	$0{,}1\cdot10^{-1}$	0,069080	0,067885
$0{,}1\cdot10^{-1}$	0,017260	0,017273	$0{,}2\cdot10^{-1}$	0,053488	0,053463	$0{,}5\cdot10^{-1}$	0,3454	0,268375
$0{,}5\cdot10^{-1}$	0,08630	0,075282	$0{,}64\cdot10^{-1}$	0,1711616	0,163831	$0{,}7\cdot10^{-1}$	0,48356	0,366879
$0{,}9\cdot10^{-1}$	0,15534	0,134851	0,104	0,278138	0,255058	$0{,}9\cdot10^{-1}$	0,621720	0,4654

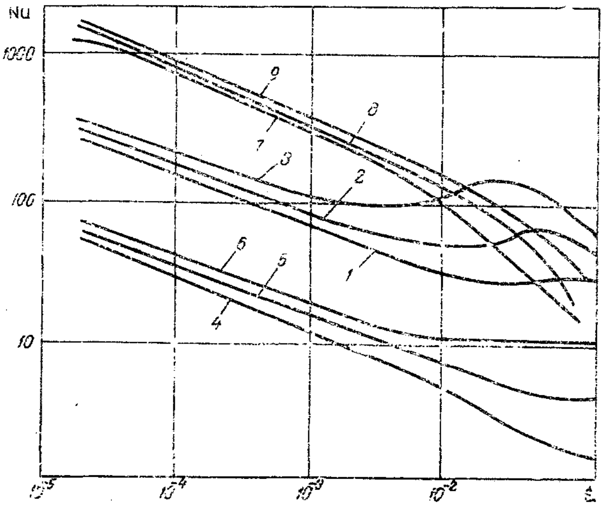

Fig. 2. Variation in Nusselt number along channel in first stage of N_2O_4 dissociation: 1, 2, 3) T_0 = 428°K; t = 1.05, 1.05, 1.1, and 1.3; 4, 5, 6) t = 1.05, 1.1, and 1.3, "frozen" values; 7, 8, 9) T = 446°K, t = 1.05, 1.1, and 1.3, respectively.

$$\omega \frac{\partial H^*}{\partial \xi} = \frac{\delta^2}{R} \cdot \frac{\partial}{\partial R}\left(R \frac{\partial H^*}{\partial R}\right) + \frac{\delta^2}{R^2} \cdot \frac{\partial^2 H^*}{\partial \varphi^2}, \tag{13}$$

where

$$H^* = \theta + \bar{Q}_{p1} C_1^*. \tag{14}$$

The heat flux at the surface of the cylinder is written as

$$-q_c = \lambda_f \frac{\partial T}{\partial r}\bigg|_{AB} + \bar{Q}_{p1} \rho D_1 \frac{\partial C_1}{\partial r}\bigg|_{AB} \tag{15}$$

or, in dimensionless form,

$$-1 = \frac{\partial \theta}{\partial R}\bigg|_{AB} + \bar{Q}_{p1} \frac{\partial C_1^*}{\partial R}\bigg|_{AB}. \tag{16}$$

Comparing (16) and (14), we have

$$\frac{\partial H^*}{\partial R}\bigg|_{AB} = -1. \tag{17}$$

The initial and boundary conditions at the lines BC, CD, and AD have the form

$$\xi = 0, \quad H^* = 0,$$

$$\frac{\partial H^*}{\partial \varphi}\bigg|_{BC,\,AD} = 0, \quad \frac{\partial H^*}{\partial n}\bigg|_{CD} = 0. \tag{18}$$

Equation (13) together with the boundary conditions (17), (18) was solved numerically with $q_c r_0/\lambda_f = 595$ on a Minsk-22 computer by the method of variable directions, the general principles of which are presented in [4, 9]. The accuracy of the solution was tested using trial functions. Suppose, for example, that we have the equation

$$L\psi = 0 \tag{19}$$

with the boundary conditions

$$\frac{\partial \psi}{\partial n}\bigg|_{\sigma} = 1, \tag{20}$$

where L is the differential operator. For the difference operator Λ, which approximates L, we have the difference equation

$$\Lambda\psi = 0, \tag{21}$$

$$\frac{\Delta\psi}{\Delta n}\bigg|_{\sigma} = 1. \tag{22}$$

For an arbitrary function f one can write

$$Lf = \varphi_1, \tag{23}$$

$$\frac{\partial f}{\partial n}\bigg|_{\sigma} = \varphi_2|_{\sigma}. \tag{24}$$

TABLE 2. Stabilized Nusselt Numbers $Nu_{f\infty}$ with Boundary Conditions of the Second Kind

t	$Nu_{f\infty}$ [5]	$Nu_{f\infty}$ [6]	$Nu_{f\infty}$ [7]	$Nu_{f\infty}$, authors' data
1,05		2,5	1,1	1,38
1,1	4,1	4	2,85	3,76
1,2	6,7	6,67	6,8	
1,3		8,5	9	8,5

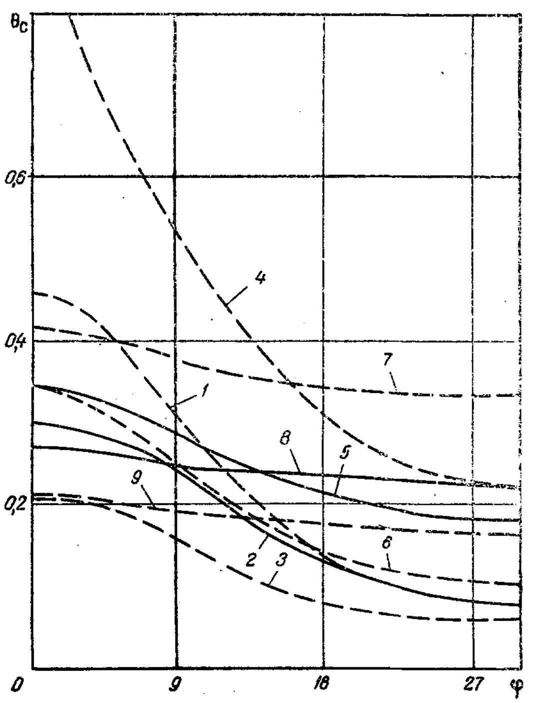

Fig. 3. Surface temperature of rod during second stage of N_2O_4 dissociation: 1, 2, 3) $t = 1.05$, $\xi = 0.26 \cdot 10^{-1}$; 4, 5, 6) $t = 1.1$, $\xi = 0.68 \cdot 10^{-1}$; 7, 8, 9) $t = 1.3$, $\xi = 0.3 \cdot 10^{-1}$; θ_{fc}, θ_c, and θ_{ec}, respectively, for each t.

It is obvious that f will satisfy the difference equation

$$\Lambda f - \varphi_1 = 0, \tag{25}$$

$$\left.\frac{\Delta f}{\Delta n}\right|_{\sigma} = \varphi_2|_{\sigma}. \tag{26}$$

Thus, one can compare the exact values of the function with those found from the difference Eqs. (25), (26). As the trial functions we chose a linear function of the form $f = \vec{a} \cdot \vec{r}$ and a nonlinear function of the form

$$f' = \vec{a} \cdot \vec{r} \, (e^{\alpha_1 \xi}, \; e^{\alpha_2 R}, \; e^{\alpha_3 \varphi}).$$

For the linear function the exact values coincided with those found from (25), (26) to the last place. For the nonlinear function in the region of point C the agreement was to 0.2%.

We determine the average mass enthalpy, which in our case coincides with the "frozen" temperature, as follows:

$$\bar{H}^* = \bar{\theta}_f = \frac{\int\limits_{\sigma} H^* \frac{U_x}{\bar{U}} \, d\sigma}{\sigma}. \tag{27}$$

On the other hand, with boundary conditions of the second kind one can write an equation for the average mass enthalpy which is obtained after integration of Eq. (13) over the cross-sectional area of the channel. This equation has the form

$$\frac{d\bar{H}^*}{d\xi} = \frac{d\theta_f}{d\xi} = 4\delta \tag{28}$$

or

$$\bar{H}^* = \theta_f = 4\delta\xi, \tag{29}$$

and the results of a calculation based on Eqs. (27) and (29) are presented in Table 1, from which it is seen that the values of $\bar{\theta}_f$ calculated from the two equations agree rather well for $\xi < 0.5 \cdot 10^{-1}$. The disagreements for larger ξ are evidently caused both by the accumulation of errors in the course of the calculations and by the calculation of the double integral of (27).

Since the first stage of N_2O_4 dissociation is an equilibrium stage the temperature field is uniquely connected with the enthalpy field. For the determination of the field of temperatures θ_e we used an experimental dependence of the enthalpy on the temperature [8] at a pressure of 150 atm, and the temperature at the channel entrance was taken as equal to 428 and 446°K.

The variation along the channel of the Nusselt numbers, determined from the hydraulic diameter, is presented in Fig. 2. The "frozen" Nusselt numbers (curves 4-6) decrease with greater distance from the channel entrance, reach their stabilized values, and remain constant after this. The stabilized values of the "frozen" Nusselt numbers $Nu_{f\infty}$ are presented in Table 2 together with the data of other authors [5-7]. For

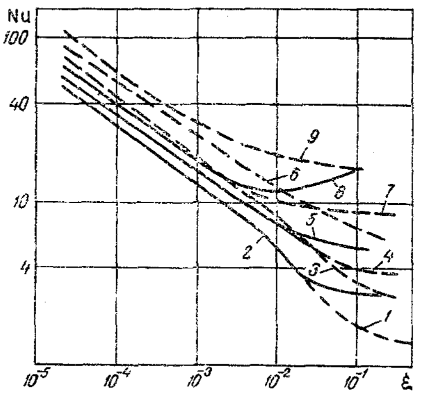

Fig. 4. Variation in Nusselt number along the channel in the second stage of N_2O_4 dissociation; 1, 2, 3) t = 1.05; 4, 5, 6) t = 1.1; 7, 8, 9) t = 1.3; Nu_f, Nu, and Nu_e, respectively, for each t.

tight bundles the results of the different authors disagree very considerably. For $t > 1.1$ the values can be considered to be in full agreement. It should be noted that in [5] the stabilized values of $Nu_{f\infty}$ are obtained with the help of the limiting transition as $Re \to \infty$, with the values of the turbulent pulsations being used as the most accurate for small Reynolds numbers. As for the comparison with experimental data on the flow of liquid metals which is made in that report, in this case the stabilized $Nu_{f\infty}$ with the laminar flow of liquid metals will always be somewhat higher than with gas flow because of the additional electron conduction of heat in metals. As for [6], the authors determined $Nu_{f\infty}$ not from the average mass temperature, but from the average temperature in the cross section, which can also lead to some overstatement of the stabilized values.

Curves 1-3 and 7-9 of Fig. 2 show the variation in Nu_e along the channel for different inlet temperatures. Curves 1-3 correspond to an inlet temperature lower than the temperature of the maximum effective heat capacity on the chosen isobar. The character of the curves is due to the fact that at the corresponding values of ξ the average surface temperature of a rod is close to the temperature of the maximum "effective heat capacity." Curves 7-9 are obtained with an inlet temperature $T_0 = 446°K$, which equals the temperature of the $c_{p\,eff}$ maximum, and as a consequence the functions $Nu_e(\xi)$ do not have extrema.

In order to determine the temperature field in the case of the second stage of nitrogen tetroxide dissociation, which, as in known, proceeds at a finite rate, the system of Eqs. (7) and (9) was solved numerically (with $Da_1 \equiv 0$, $q_c r_0/\lambda_f = 595$, $T_0 = 500°K$, $C_{40} = 0.001$, $P = 10$ atm, and a noncatalytic cylinder surface, by the same method of variable directions) with the boundary conditions

$$\begin{gathered}
\xi = 0, \quad \theta = 0, \quad C_4^* = 0, \\
\left.\frac{\partial\theta}{\partial R}\right|_{AB} = -1, \quad \left.\frac{\partial C_4^*}{\partial R}\right|_{AB} = 0, \\
\left.\frac{\partial\theta}{\partial\varphi}\right|_{BC,\,AD} = \left.\frac{\partial C_4^*}{\partial\varphi}\right|_{BC,\,AD} = 0, \\
\left.\frac{\partial\theta}{\partial n}\right|_{CD} = \left.\frac{\partial C_4^*}{\partial n}\right|_{CD} = 0.
\end{gathered} \tag{30}$$

The temperature variation on the surface of a rod is presented in Fig. 3. Since the effect of the chemical reaction is manifested at a certain distance which depends on the lattice spacing, the temperatures at the rod surface are shown for different values of ξ. The effect of the chemical reaction on the heat exchange is manifested in particular in a marked decrease in the temperature variation of the surface. This is due to the additional heat transfer because of the concentration diffusion from the "stagnant zone" to the axis of symmetry of the channel.

In the case of tight bundles (Fig. 3, curves 1-3) the temperature in the "stagnant zone" is close to the equilibrium temperature, whereas it coincides with the "frozen" temperature in the region of the axis of symmetry of the channel. The fact that equilibrium is established in the "stagnant zone" while the flow can remain "frozen" in the region of the axis of symmetry leads to the fact that cases are possible where the temperature variation for a chemical reaction proceeding at a finite rate will be smaller than for an equilibrium reaction (Fig. 3, curves 4-6). For spread bundles with $t \geq 1.3$ the effect of the neighboring rods is not very great and the temperature assumes an intermediate values between the "frozen" and equilibrium temperatures (Fig. 3, curves 7-9), with the curves being about equidistant, which indicates that equilibrium in the stream is reached more uniformly over the perimeter than for tight bundles.

If the chemical reaction proceeds with a finite rate then the Nusselt numbers in the initial section of the channel coincide with the "frozen" Nu, since the time the gas remains in the channel is insignificant (Fig. 4). The difference from Nu_f becomes ever more substantial with greater distance from the entrance and at certain values of ξ the Nusselt numbers reach their equilibrium values. Since the time the gas remains in the channel increases with an increase in the spacing, in spread bundles equilibrium is reached at smaller distances from the entrance than in the case of tight bundles (Fig. 4, curves 2 and 3, 5 and 6, and 8 and 9).

In conclusion, we note that in the case of chemical reactions the heat exchange proceeds considerably more intensively than with the flow of chemically inert substances, with the maximum intensity being reached in the case of equilibrium flow. Moreover, with longitudinal flow of a chemically reacting stream over bundles of heated cylinders the temperature variation over the perimeter of a cylinder is considerably reduced.

NOTATION

t	is the spacing of rods;
r_0	is the radius of cylinders;
d_h	is the hydraulic diameter;
$R = r/r_0$	is the dimensionless radius;
$\xi = 1/RePr \cdot x/d_n$	is the dimensionless longitudinal coordinate;
$\theta = (T-T_0)/q_c r_0/\lambda_f$	is the dimensionless temperature;
$C_k^* = C_k - C_{k0}$	is the relative concentration of component k;
$H^* = (H-H_0 \cdot q_c r_0/\lambda_f)/c_{pf}$	is the dimensionless enthalpy;
j_k	is the mass flux of component k, kg/m^2 · sec;
J_k	is the mass source of k-th component, kg/m^3· sec;
I_l	is the rate of reaction l, kmole/m· sec;
m_k	is the molecular weight of component k, kmole/kg;
Q_{pl}	is the calorific effect of reaction l, kJ/kmole;
$\delta = d_h/r_0$;	
U_x	is the longitudinal velocity component;
$\bar{U}$	is the average mass velocity;
$Re = Ud_h/\nu$;	
$Pr = \nu/a$;	
$Le_k = \rho D_k c_{pf}/\lambda_f$;	
$Da_k = J_k d_g^2/\rho D_k$	is the Damkeller number;
$Q_{pl} = Q_{pl}/m_k c_{pf} q_c r_0/\lambda_f$;	
q_c	is the specific heat flux, kW/m^2;
σ	is the cross-sectional area.

Indices

f	are the "frozen" values;
e	are the equilibrium values;
c	are the parameters at surface of cylinder;
0	are the parameters at channel entrance;
k, k-th	is the k-th component;
l, l-th	is the Z-th reaction;
1) N_2O_4; 2) NO_2; 3) NO; 4) O_2;	
∞	are the stabilized values of parameters.

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