A METHOD OF COMPUTING HEAT TRANSFER COEFFICIENT IN THE FLOW OF A CHEMICALLY REACTING N_2O_4 GAS

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A criterial relation is derived which connects the heat transfer coefficient with the difference in the concentrations of the O_2 component at the wall and in the flow. A method of determining the concentration difference is proposed. A comparison with the experimental data shows that the proposed method gives satisfactory results in a wide range of pressures and temperatures.

Assuming that the turbulent heat and mass transports are similar and that the "frozen-in" Lewis number is equal to unity, the equation of conservation of energy for a chemically active gas can be written in the form of the corresponding equation for an inert gas [1] and the solutions of these equations for appropriate boundary conditions will coincide:

$$H(x, R) = \theta_f(x, R),$$

$$\theta = \frac{T_f - T_{\text{in}}}{q_c r_0/\lambda_f}, \quad H = \frac{h - h_{\text{in}}}{c_{pf} q_c r_0/\lambda_f}.$$

Therefore Nusselt number for a chemically inert gas

$$\mathrm{Nu}_f = \frac{q_c d}{\lambda_f (T_{fc} - T_{f0})} = \frac{2}{\theta_{fc} - \theta_{f0}}$$

and for a chemically active gas referred to the enthalpy difference at the wall and in the flow

$$\mathrm{Nu}(h) = \frac{q_c d c_{pf}}{\lambda_f (h_c - h_0)} = \frac{2}{H_c - H_0},$$

will be equal

$$\mathrm{Nu}_f = \mathrm{Nu}(h). \tag{1}$$

The ratio of Nusselt numbers for a chemically reacting gas

$$\mathrm{Nu} = \frac{q_c d}{\lambda_f (T_c - T_0)} = \frac{2}{\theta_c - \theta_0}$$

and for a chemically inert gas will be, taking into account (1), the following:

$$\frac{\mathrm{Nu}}{\mathrm{Nu}_f} = \frac{\mathrm{Nu}}{\mathrm{Nu}(h)} = \frac{h_c - h_0}{c_{pf}(T_c - T_0)} = \frac{1}{c_{pf}(T_c - T_0)} \int_{T_0}^{T_c} c_{peff}\, dT = \frac{c^0_{peff}}{c_{pf}}.$$

On the other hand

$$c^0_{peff} = \frac{1}{\Delta T} \int_{T_0}^{T_c} c_{peff}\, dT = \frac{1}{\Delta T} \int_{T_0}^{T_c} \left(c_{pf} + \sum_{j=1}^{n} \frac{Q_{pj}}{m_j a_{jj}} \frac{dc_j}{dT} \right).$$

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According to computations c_{pf} changes very insignificantly in a wide range of temperatures. For example, in the range 300-1000°K c_{pf} changes from 0.21 to 0.26 kcal/kg · deg. Therefore it can be taken to be constant and equal to the mean value in the temperature range T_0-T_c.

Hence

$$c^0_{peff} = c_{pf} + \sum_{j=1}^{n} \frac{Q_{pj}}{m_j a_{jj}} \frac{\Delta c_j}{\Delta T},$$

and for the reaction proceeding in accordance with the scheme

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

we obtain

$$\frac{Nu}{Nu_f} = \frac{c^0_{peff}}{c_{pf}} = 1 + \frac{Q_{pI}}{m_1} \frac{c_{10} - c_{1c}}{c_{pf}(T_c - T_0)} + \frac{Q_{pII}}{m_4} \frac{c_{4c} - c_{40}}{c_{pf}(T_c - T_0)}. \tag{2}$$

Equation (2) enables one to compute the heat transfer coefficient in the turbulent channel flow of the mixture in chemical equilibrium ($N_2O_4 \rightleftarrows 2NO_2$) and nonequilibrium ($2NO_2 \rightleftarrows 2NO + O_2$). In the first case the following equation is used for determining the relative concentration of the N_2O_4 component at the wall [7]:

$$c_{1c} = \frac{m_1}{m_2} \frac{\rho}{K_{cI}(T_c)} c^2_{2c}.$$

The results of an experimental investigation of heat transfer in the turbulent flow of an equilibrium dissociating mixture $N_2O_4 \rightleftarrows 2NO_2$ in a circular tube have been analyzed for the pressure range P = 10-85 atm and for the values of Reynolds number Re = 10^4-$2 \cdot 10^5$. It was found that formula (2) describes the experimental points with a maximum scatter of 15%. As the results showed, this formula is applicable even in the pressure range P = 120-150 atm. In the case of the second nonequilibrium dissociation stage

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

the formula for computing the concentration of the O_2 component is obtained in the following way.

The equation of mass conservation for the k-th component can be written in the following form under the assumption that the diffusion coefficient and the density are constant, and Prandtl number is equal to unity:

$$\frac{Re}{2} \omega Sc \frac{\partial c_k}{\partial x} = \frac{1}{R} \frac{\partial}{\partial R} \left[R \left(1 + \frac{\mu_T}{\mu} Sc \right) \frac{\partial c_k}{\partial R} \right] + Da_k, \tag{3}$$

$$\omega = \frac{w_x}{w_0}, \quad Da_k = \frac{I_k r_0^2}{\rho D_k}.$$

Integrating Eq. (3) over R from 0 to 1 and putting $\partial c_k / \partial R|_1 = 0$, we obtain

$$\frac{Re}{2} Sc \frac{\partial c_{k0}}{\partial x} = Da_{k0}. \tag{4}$$

Assuming that $\partial c_k / \partial x \approx \partial c_{k0} / \partial x$ [3] and making use of (4) we obtain the following equation for the concentration difference:

$$c_{kc} - c_k = \int_0^1 \frac{\int_0^R (\omega Da_{k0} - Da_k) R dR}{\left(1 + \frac{\mu_T}{\mu} Sc \right) R} dR. \tag{5}$$

We introduce the definition

$$c_{kc} - c_{k0} = 2 \int_R^1 \omega (c_{kc} - c_k) R dR.$$

Making use of (5) we can now write

$$c_{kc} - c_{k0} = 2 \int_0^1 \omega \left[\int_R^1 \frac{\int_0^R (\omega Da_{k0} - Da_k) R dR}{\left(1 + \frac{\mu_T}{\mu} Sc \right) R} dR \right] R dR. \tag{6}$$

Putting $\omega = 1$ and remembering that $0.5 \le \mathrm{Sc} \le 1$ we have

$$\frac{\mu_T}{\mu}\mathrm{Sc} \gg 1,$$

We apply the method of integration of a product to Eq. (6) twice. Then for the second nonequilibrium dissociation stage we have

$$c_{4c} - c_{40} = -\frac{\mathrm{Da}_{40}}{\chi}\left[\Theta\int_R^1 R\exp\left(\frac{\gamma}{T_0} - \frac{\gamma}{T_c}\right)\ln|\delta - R|\left(\frac{c_2}{c_{20}}\right)^2 - \Theta\int_0^1 R\left(\frac{c_4}{c_{40}}\right)^3 \ln|\delta - R|\,dR + \frac{3}{4}\right],$$

$$\mathrm{Sc}\frac{\mu_T}{\mu} = \chi(\delta - R)R, \quad \chi = a\,\mathrm{Re}\sqrt{\xi/32}\,\mathrm{Sc}, \quad \xi = \frac{0{,}316}{\mathrm{Re}^{0{,}25}}[4-6],$$

$$a = 0.39, \quad \Theta = \frac{m_4 J_{\mathrm{II}}^{\mathrm{d}}}{I_{40}}, \quad \tilde{\Theta} = \frac{m_4 J_{\mathrm{II}}^{\mathrm{rev}}}{I_{40}}, \quad I_4 = m_4[J_{\mathrm{II}}^{\mathrm{d}} - J_{\mathrm{II}}^{\mathrm{rev}}],$$

$$J_{\mathrm{II}}^{\mathrm{d}} = \frac{\rho^2}{m_2^2}K_{\mathrm{cII}\partial}c_2^2, \quad J_{\mathrm{II}}^{\mathrm{rev}} = 4\frac{K_{\mathrm{cII}\partial}}{K_{\mathrm{cII}}}\frac{\rho^3 c_4^3}{m_4^3}, \tag{7}$$

$$K_{\mathrm{cII}\partial} = 10^{8{,}97}\exp\left(-\frac{25800}{RT}\right), \quad K_{\mathrm{cII}} = \frac{K_{p\mathrm{II}}}{R'T},$$

$$\ln K_{p\mathrm{II}} = -0.5845\ln(T\cdot 10^{-4}) + 12.5862\cdot 10^4\frac{1}{T^2} - 147.088\cdot 10^2\frac{1}{T}$$
$$+ 17.5121 - 0.3079\cdot 10^{-4}T - 1.60117\cdot 10^{-8}T^2 - 0.1183\cdot 10^{-12}T^3[7].$$

Let us evaluate the integrals occurring in (7):

$$\int_0^1 R\left(\frac{c_2}{c_{20}}\right)^2 \exp\left(\frac{\gamma}{T_0} - \frac{\gamma}{T_c}\right)\ln|\delta - R|\,dR = \int_0^1 \frac{R\ln|\delta - R|}{\frac{\gamma}{x_0 T^2}\frac{dT}{dR}}e^{x_0 x}dx. \tag{8}$$

Here

$$\frac{c_2}{c_{20}} \approx 1; \quad x = \frac{1 - \frac{T_0}{T}}{1 - \frac{T_0}{T_c}}; \quad x_0 = \frac{\gamma}{T_0}\left(1 - \frac{T_0}{T_c}\right).$$

We shall approximate the integrand in the following way:

$$\frac{R\ln|\delta - R|}{\frac{\gamma}{x_0 T^2}\frac{dT}{dR}} \approx Ax^5 - x. \tag{9}$$

We can determine A, for example, from the condition of equality of the right and left hand sides of Eq. (9) for $x = R = 1$. For the investigated range of parameters $q = 1.4\text{–}5.5\cdot 10^2$, $\mathrm{Re} = 0.2\text{–}2\cdot 10^5$ A was found to be approximately equal to 1. Then integral (8) becomes

$$\int_0^1 (x^5 - x)e^{x_0 x}dx = e^{x_0}f_1,$$

where

$$f_1 = \frac{4}{x_0^2}\left(1 - \frac{5}{x_0} + \frac{15}{x_0^2} - \frac{30}{x_0^3} + \frac{30}{x_0^4} + \frac{e^{-x_0}}{4} - \frac{30e^{-x_0}}{x_0^4}\right).$$

Next

$$f_2 = \int_0^1 R\left(\frac{c_4}{c_{40}}\right)^3 \ln|\delta - R|\,dR = \int_0^1 R\left(\frac{c_{4\infty}}{c_{40}}\right)^3 \ln|\delta - R|\,dR$$

$$-3\int_0^1 R\left(\frac{c_{4\infty}}{c_{40}}\right)^2 \frac{c_{4\infty} - c_4}{c_{40}}\ln|\delta - R|\,dR + 3\int_0^1 R\frac{c_{4\infty}}{c_{40}}\left(\frac{c_{4\infty} - c_4}{c_{40}}\right)^2 \ln|\delta$$

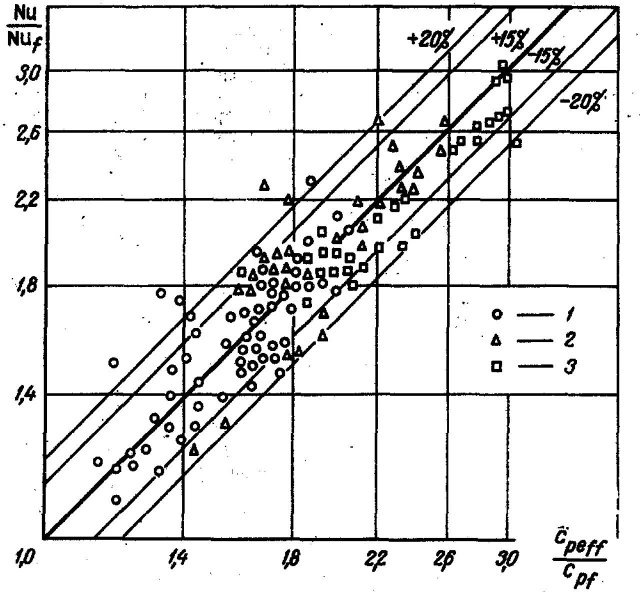

Fig. 1. A comparison of the results of computation by formulas (2), (10) with experimental data in the range of parameters P = 11.5-150 atm, Re = 0.3-2 · 10^5, T_0 = 500-800°K, T_c = 559-900°K [1) P = 11.5-30 atm; 2) 40-85; 3) 120-150]. The ratio c^0_{peff}/c_{pf} is plotted on the abscissa.

$$-R|\,dR-\int_0^1 R\left(\frac{c_{4\infty}-c_4}{c_{40}}\right)^3 \ln|\delta-R|\,dR.$$

Remembering that

$$\left(\frac{c_{4\infty}}{c_{40}}\right)^3=\left(\frac{1-\frac{m_1}{m_4}c_{4\infty}}{1-\frac{m_1}{m_4}c_{40}}\right)^2\cdot\frac{K_{c\text{II}\partial}}{K^0_{c\text{II}\partial}},$$

we obtain

$$f_2=-\left(\frac{c_{4\infty}}{c_{40}}\right)^3\left[f_1(x_0)-3\left(1-\frac{c_{4c}}{c_{4c\infty}}\right)f_1\left(\frac{2}{3}x_0\right)+3\left(1-\frac{c_{4c}}{c_{4c\infty}}\right)^2 f_1\left(\frac{x_0}{3}\right)-\frac{3}{4}\left(1-\frac{c_{4c}}{c_{4c\infty}}\right)^3\right].$$

Thus we get

$$c_{4c}-c_{40}=\frac{1}{\chi}\left(\mathrm{Da}^{\mathrm{d}}_{40}\,f_1'-\mathrm{Da}^{\mathrm{rev}}_{40}\,f_2'\right),$$

where

$$f_1'=e^{x_0}f_1-\frac{3}{4};\quad f_2'=-f_2-\frac{3}{4}.$$

Using the above method of computing the heat transfer coefficient we analyzed the results of experimental investigations carried out at the Nuclear Energetics Institute of the Academy of Sciences of the BSSR [8, 9] (see Fig. 1). The scatter of the points is ±20% and the root mean square error is 5%. The average values of the quantities were calculated in accordance with the recommendations of [10].

NOTATION

h	is the specific enthalpy, kcal/kg;
τ	is the time, sec;
q	is the heat flux density, kcal/m^2 · sec;
$c_k = \rho_k/\rho$	is the relative partial density of the k-th component;

ρ	is the density of the multicomponent mixture, kg/m^3;
I_k	is the source of the k-th component of the mixture, $kg/m^3 \cdot sec$;
D_k	is the diffusion coefficient of the multicomponent mixture, m^2/sec;
λ	is the thermal conductivity, $kcal/m^2 \cdot sec$;
T	is the absolute temperature, °K;
Le	is the Lewis number;
c_p	is the specific heat at constant pressure, $kcal/kg \cdot deg$;
w	is the velocity of the fluid, m/sec;
Re	is the Reynolds number;
Pe	is the Peclet number;
Sc	is the Schmidt number;
$\mu(\mu_T)$	is the coefficient of dynamic (turbulent) viscosity, $kg/m \cdot sec$;
$\delta = 1-\delta^*/r_0$;	
δ^*	is the thickness of the laminar sublayer, m;
J_{II}^{d}, J_{II}^{rev}	are the direct and reverse reaction rates of the second stage of decomposition of N_2O_4, $kg/m^3 \cdot sec$;
$\gamma = E/R$	is a coefficient, deg;
E	is the activation energy, kcal/kmole;
R	is the universal gas constant, $kcal/kmole \cdot deg$;
R'	is the universal gas constant, $m^3 \cdot atm/kmole \cdot deg$;
$K_{cII\partial}$, K_{cII}	are the rate constants of dissociation, $liter/mole \cdot sec$ and equilibrium, mole/liter, of the second stage of decomposition of N_2O_4, respectively;
m_k	is the mass of the k-th component;
Q_{pI}, Q_{pII}	are the heat effects of the first and second stage of reaction, kcal/kmole.

Subscripts

k	denotes the k-th component of the mixture;
f	denotes the "frozen-in" component;
eff	denotes the "effective" characteristics;
c	denotes the wall parameters;
o	denotes the flow parameters;
in	denotes the value of the parameters at the entrance to the channel;
∞	denotes the value of the parameters in the case of equilibrium reaction;
1	denotes N_2O_4;
2	denotes NO_2;
3	denotes NO;
4	denotes O_2;
d, rev	denote the direct and reverse reactions;
I	denotes the first stage of the reaction;
II	denotes the second stage.

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