METHODS OF USING A DIGITAL COMPUTER TO CALCULATE THE HEAT-TRANSFER COEFFICIENTS OF PERIODIC HEAT EXCHANGERS

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We propose a method of calculating the heat-transfer coefficients that is based on comparison of the operational data and the equations of heat-transfer dynamics.

In many of the chemical processes taking place in apparatus of periodic operation there is a rather broad range of variation in temperature (100-300°C), and the variations in the heat-transfer coefficients thus reach significant magnitudes. For example, in the production of certain types of synthetic resins the heat-transfer coefficients vary by factors of 2.5-3.5 [1, 2].

This makes absolutely clear the need for consideration of the effect of temperature in the heat-transfer coefficients whose determination is best accomplished with application of the method of dynamic characteristics [2].

The dynamics of heat exchange in periodic equipment can be described with sufficient accuracy [1-3] by a nonlinear differential equation of the form

$$a(y)\frac{dy(\tau)}{d\tau} + by(\tau) = x(\tau). \tag{1}$$

The analytical derivation of the dynamics equation has demonstrated [1, 2] that for the various heat-exchange methods $a(y)$ and $x(\tau)$ have the form:

from the saturated vapors of the heat carriers

$$a(y) = \frac{Mc(y)}{k(y)F}, \tag{2}$$

$$x(\tau) = t_s, \tag{2a}$$

from single-phase heat-transfer media

$$a(y) = \frac{Mc(y)}{W\left[1 - \exp\left(-\frac{k(y)F}{W}\right)\right]}, \tag{3}$$

$$x(\tau) = t'_h, \tag{3a}$$

from the wall of the apparatus

$$a(y) = \frac{Mc(y)}{\alpha(y)F}, \tag{4}$$

$$x(\tau) = t_w. \tag{4a}$$

From (2)-(4) it is not difficult to determine the coefficients of heat transfer* and of heat exchange, these being functions of $y(\tau)$. The heat capacity as a function of temperature, i.e., $c(y)$, must be known in

*It is easy to make the transition from the heat-transfer coefficients to the heat-exchange coefficients by means of the Wilson method [4].

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advance and for the majority of cases can be approximated by the linear relationship

$$c(y) = P_0 + P_1 y, \tag{5}$$

whose coefficients P_0 and P_1 are found from the known tabulated values by the method of least squares.

Consequently, the problem of calculating the heat-exchange coefficients reduces to the determination of $a(y)$, which is best accomplished by an experimental–analytical method whose essence involves the following. Let us set up the following experiment in the equipment being investigated, and for the time interval $[0, \tau_n]$ let us write the functions $x_{ex}(\tau_i)$ and $y_{ex}(\tau_i)$, together with the random perturbations imposed on these. These functions are found most frequently in a table for the values of $x_{ex}(\tau_i) = x_{exi}$; $y_{ex}(\tau_i) = y_{exi}$ $(i = 0, 1, 2, \ldots, n)$.

Further, let us compile the functional

$$\Phi = \int_0^{\tau_n} [y_{ex}(\tau) - y(\tau)]^2 \, d\tau \tag{6}$$

or the function

$$\Phi = \sum_{i=0}^{n} [y_{ex}(\tau) - y(\tau)]^2. \tag{6a}$$

In these expressions $y(\tau)$ is the solution of (1) for $x(\tau) = x_{ex}(\tau)$, $0 \leq \tau \leq \tau_n$, and $y(0) = y_{ex}(0)$. In (1) we have to choose the function $a(y)$ for which the functional attains its minimum. Most probably, $\Phi > 0$, since (1) describes the dynamics of the apparatus only approximately. If we can find $a(y)$ from this condition, Eq. (1) will best describe the heat-exchange process of a specific piece of equipment (within the framework of similar relationships), since with $y_{ex}(\tau)$ we take into consideration all of that piece of equipment's individual features, e.g., deposition on the walls, etc.

The formulated problem is a variational problem with a conditional extremum, and the use of the Lagrange method for its solution is made difficult by the absence in (6) of the extremal $a(y)$ and its first derivative. We will therefore offer two methods below for an approximate determination (using a digital computer) of the function $a(y)$ from the experimentally found values of $x_{ex}(\tau)$ and $y_{ex}(\tau)$.

Let us assume that $x_{ex}(\tau) = \tilde{x}_{ex}(\tau) + z_x(\tau)$ and $y_{ex}(\tau) = \tilde{y}_{ex}(\tau) + z_y(\tau)$, where $z_x(\tau)$ and $z_y(\tau)$ are normally distributed perturbations with zero mathematical expectations; $\tilde{x}_{ex}(\tau)$ and $\tilde{y}_{ex}(\tau)$ are smooth monotonic functions. The sources for the appearance of $z_x(\tau)$ and $z_y(\tau)$ are the errors in the measurement of $\tilde{x}_{ex}(\tau)$ and $\tilde{y}_{ex}(\tau)$ during the course of the experiments, as well as random fluctuations in the observed parameters, the effect of factors for which no provision had been made, etc. Let us approximate the tabulated functions x_{exi}, y_{exi} $(i = 0, 1, 2, \ldots, n)$ by the orthogonal Chebyshev polynomials with a weighting function equal to unity, and we find

$$\tilde{x}_{ex}(\tau) = \sum_{\lambda=0}^{m} c_\lambda \varphi_\lambda(\tau) = \sum_{\lambda=0}^{m} r_\lambda \tau^\lambda, \tag{7}$$

$$\tilde{y}_{ex}(\tau) = \sum_{\lambda=0}^{k} c_\lambda \varphi_\lambda(\tau) = \sum_{\lambda=0}^{k} d_\lambda \tau^\lambda. \tag{8}$$

It is obvious that $\varphi_\lambda(\tau)$ are polynomials of degree λ, while c_λ are constant Fourier coefficients calculated from the familiar formulas of (5). Then r_λ and d_λ are easily found in terms of c_λ and $\varphi_\lambda(\tau)$, after cancellation of similar terms. The values of m and k are chosen so as to filter out the perturbations $z_x(\tau)$ and $z_y(\tau)$ and not to distort the significant singularities of $\tilde{x}_{ex}(\tau)$ and $\tilde{y}_{ex}(\tau)$. For this we can use one of two methods.

Let us specify the value $m = m_1$ (usually m_1 is a small number, e.g., $m_1 = 1$), and we will calculate

$$D[x(m_1)] = \frac{1}{n+1} \sum_{i=0}^{n} [x_{ex\,i} - \tilde{x}_{ex}(\tau_i)]^2. \tag{9}$$

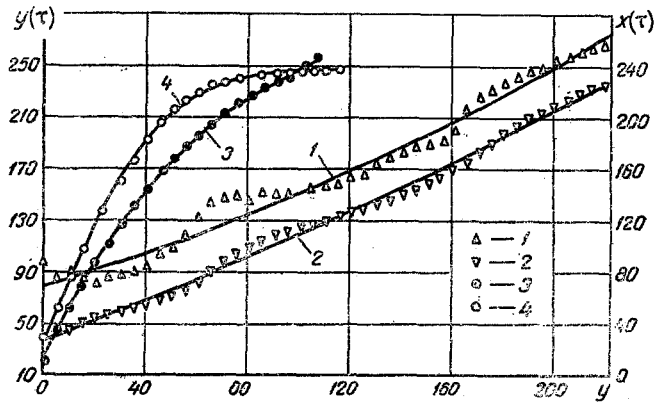

Fig. 1. Relationship giving x and y as functions of time: 1) $x_I(\tau)$; 2) $y_I(\tau)$; 3) $y_{II}(\tau)$; 4) $y_{III}(\tau)$.

We will then assume $m_2 = m_1 + 1$, we will find $D[x(m_1 + 1)]$, and we will compare the dispersions. If $D[x(m_1)]$ is substantially larger than $D[x(m_1 + 1)]$, for example, by 20-40%, we assume m is equal to $m_1 + 2$, we determine $D[x(m + 2)]$, and the latter is compared with the dispersion for $D[x(m + 1)]$. With a slight difference between the values of $D[x(m_1)]$ and $D[x(m_1 + 1)]$ we take the quantity m_1 for m.

The second method of finding m or k will be used if $z_x(\tau)$ and $z_y(\tau)$ are governed exclusively by the measurement errors. If Δx is the greatest error in the measurement of $\tilde{x}_{ex}(\tau)$ – determined by the class of the instrument – we have the relationship $D[x(m)] \leq (\Delta x/3)^2$, from which we can find the value of m.* The orthogonality of (7) and (8) simplifies the problem of calculating r_λ and d_λ in chosing m and k.

Further, assuming that $x(\tau) \approx \tilde{x}_{ex}(\tau)$ and $y(\tau) \approx \tilde{y}_{ex}(\tau)$, we find $a(\tau)$ from (1) as a function of time:

$$a(\tau) = \frac{\sum_{\lambda=0}^{m} r_\lambda \tau^\lambda - b \sum_{\lambda=0}^{k} d_\lambda \tau^\lambda}{\sum_{\lambda=1}^{k} \lambda d_\lambda \tau^{\lambda-1}}. \tag{10}$$

The denominator in (10) is found by the differentiation operation, which here does not result in the appearance of significant errors, since the perturbation $z_y(\tau)$ has been separated from $\tilde{y}_{ex}(\tau)$.

Substantial errors arise only when $\tilde{y}_{ex}(\tau) \approx$ const at certain segments. These segments are usually found at the beginning and end of the interval $[0, \tau_n]$. To reduce the error in the determination of $a(\tau)$ we must eliminate the segments with $y_{ex}(\tau) \approx$ const from our examination during the course of the calculation.

Comparing the values of $a(\tau_i)$ with $y_{ex}(\tau_i)$, we obtain

$$a(y) = \sum_{\lambda=0}^{l} q_\lambda y^\lambda, \tag{11}$$

where the coefficients q_λ are found by the method of least squares.

The accuracy in the determination of $a(y)$ by this method, as a rule, is completely acceptable for engineering calculations. However, our assumptions to the effect that the bounds of the mathematical expectations $z_x(\tau)$ and $z_y(\tau)$ are equal to zero, while $y(\tau) \equiv \tilde{y}_{ex}(\tau)$ when $0 \leq \tau \leq \tau_n$, are rather rigid, and what is most important, frequently cannot be verified. These can be found in the determination of $a(y)$ by the second method, i.e., an iteration method.

Let us expand $a(y)$ in series in powers of y, i.e.,

$$a(y) = \sum_{\lambda=0}^{l} q_\lambda y^\lambda. \tag{12}$$

We will specify the values of l, assuming usually that $l = 3$-5. Having substituted (12) into (1) and having found the solution $y(\tau)$ for $x(\tau) = x_{ex}(\tau)$ by some numerical method, we determine the magnitude of Φ. Expressions (6) or (6a) have now been turned into a function of the unknown variables q_λ. Consequently,

*The determination of k is handled in a similar fashion.

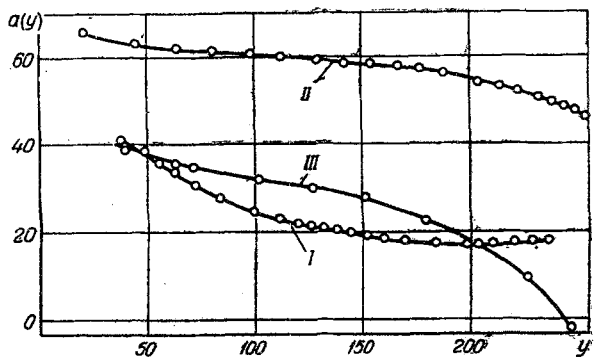

Fig. 2. The function $a(y)$: I) $a_I(y)$; II) $a_{II}(y)$; III) $a_{III}(y)$.

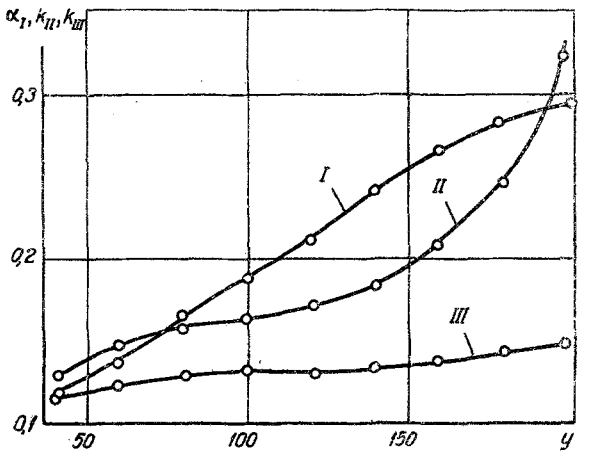

Fig. 3. Temperature relationship for the heat-exchange coefficients: I) $\alpha_I(y)$; II) $k_{II}(y)$; III) $k_{III}(y)$.

to determine $a(y)$ we have to find the set q_λ for which the function Φ attains the local conditional minimum. The minimization problem is solved by a gradient method. We find the point of minimum Φ by the iteration formula for [6], successively for each j-th iteration (j = 0, 1, 2, ..., n) with the iteration interval h

$$q_\lambda^{j+1} = q_\lambda^j - h \frac{\partial \Phi / \partial q_\lambda}{\sqrt{\sum_{\lambda=0}^{b} (\partial \Phi / \partial q_\lambda)^2}} . \tag{13}$$

The partial derivatives $\partial\Phi/\partial q_\lambda$ are calculated by a different method. To speed up the process of finding the minimum Φ we have to assume the q_λ from (11) as the initial approximation of q_λ^0, thus simultaneously determining the choice of the order of the polynomials. Since both methods of determining $a(y)$ use the same initial data, it is expedient to compile a single calculation program for the digital computer.

Let us explain the above method in an example of determining $a(y)$ for reactors: with an induction heating method (curves $x_I(\tau)$ and $y_I(\tau)$, see Fig. 1); with a jacket heated by the saturated vapors of a high-temperature organic heat carrier, i.e., ditolylmethane ($x_{II}(\tau)$ = const = 300°C, $y_{II}(\tau)$, see Fig. 1); with an external coil heated by a single-phase liquid TAS-190 organic silicon heat carrier ($x_{III}(\tau)$ = const = 250°C, $y_{III}(\tau)$, see Fig. 1).

We have thus presented the following methods of achieving heat exchange with the material in the apparatus: heat exchange with the wall of the apparatus, the transfer of heat from the film condensate, and the transfer of heat from a single-phase liquid heat carrier.

Let us present the experimentally derived data as polynomials of the form of (7) and (8) with $m_1 = k_1 = 2$ and $m_2 = k_2 = 3$. Since $D[x_1(m_1)] = 77.98$ [°C^2], and $D[x_1(m_2)] = 77.47$ [°C^2], in the interval $0 \leq \tau \leq 220$ min we can approximate $\tilde{x}_I(\tau)$ by the expression

$$\tilde{x}_I(\tau) = 70.548 + 0.592\tau + 0.13 \cdot 10^{-2} \tau^2 . \tag{14}$$

Similarly, for $y_I(\tau)$ we have $[D(y_1(k_1)] = 19.083$ [°C^2] and $D[y_1(k_2)] = 17.11$ [°C^2], and therefore, for the same time interval

$$\tilde{y}_I(\tau) = 39.362 + 0.730\tau + 0.728 \cdot 10^{-3} \tau^2 . \tag{15}$$

In similar fashion, we obtain the polynomials for the remaining two cases:

$$\tilde{y}_{II}(\tau) = 21.898 + 4.286\tau - 0.0273\tau^2 + 0.707 \cdot 10^{-4} \tau^3 \tag{16}$$

when $0 \leqslant \tau \leqslant 105$ min,

$$\tilde{y}_{III}(\tau) = 36.559 + 5.566\tau - 0.0444\tau^2 + 0.1279 \cdot 10^{-3} \tau^3 \tag{17}$$

when $0 \leqslant \tau \leqslant 115$ min.

Having differentiated (15) with respect to τ and having substituted $\tilde{y}_I(\tau)$, $\dot{y}_I(\tau)$, and $\tilde{x}_I(\tau)$ into (10), we calculate $a(\tau_i)$ at the point τ_i for $\Delta\tau = \tau_{i+1} - \tau_i = 5$ min, $i = 0, 1, \ldots, 45$. It is then easy to find the graphical function $a(y)$, plotting the values of $y_{Iex}(\tau_i)$ and $a_I(\tau_i)$ along the axes (see curve I in Fig. 2). We approximate the table of correspondences $\| y_{Iex}(\tau_i),\ a_i(\tau_i) \|$ by the polynomial

$$a_I(y_I) = 52.37427 - 0.366704\, y_I + 0.9506 \cdot 10^{-3} y_I^2. \tag{18}$$

The chosen degree of the polynomial becomes understandable from comparison of the dispersions

$$D[a_I(1)] = 9.94\ [°C^2],\ D[a_I(2)] = 0.563\ [°C^2],\quad D[a_I(3)] = 0.394\ [°C^2].$$

For the two remaining apparatuses, we obtain the graphical relationships in a similar manner (see curves II and III in Fig. 2), as well as the approximation polynomials:

$$a_{II}(y) = 68.33467 - 0.152847\, y_{II} + 0.1071 \cdot 10^{-2} y_{II}^2 - 0.3184 \cdot 10^{-5} y_{II}^3, \tag{19}$$

$$a_{III}(y) = 50.0595 - 0.369444\, y_{III} + 0.2752 \cdot 10^{-2} y_{III}^2 - 0.8561 \cdot 10^{-5} y_{III}^3 \tag{20}$$

with $D[a_{II}(3)] = 0.48\ [°C^2]$ and $D[a_{III}(3)] = 1.398\ [°C^2]$.

The function $a_{III}(y)$ for $243.5 \leq y_{III}(\tau) \leq 247.1$ is negative, and as was explained above, this is not a physical paradox – a negative heat-exchange coefficient – but is a result exclusively of an error in differentiation, since beginning with $\tau = 85$ min, $y_{III}(\tau)$ becomes virtually constant. Since the accuracy with which the heat-exchange coefficient is calculated about the zero value of $y_{III}(\tau)$ is low, it is advisable to reduce the interval for the specification of the experimental data and of functions (17) and (20) to [0, 85] min, eliminating the points from $y_{III}(90)$ to $y_{III}(115)$ from our consideration, since these are virtually indistinguishable from one another.

The coefficients for the derived equations (18)-(20) are further refined by the gradient method. To calculate the partial derivatives we have test increments Δq_λ, amounting to 1-2% of the found values of q_λ; the quantity h amounts to 3-5% of q_λ^0 for $\Phi(q_\lambda^{j+1}) < \Phi(q_\lambda^j)$ and begins to diminish by half with each interval as the inequality is disrupted; Eq. (1) was integrated on the computer by the Runge–Kutta method with a variable interval. The initial values of the function Φ, respectively, amounted to

$$\Phi_I(q_\lambda^0) = 90.175;\ \Phi_{II}(q_\lambda^0) = 38.559 \text{ and } \Phi_{III}(q_\lambda^0) = 581.83.$$

After descent from q_λ^0 on the basis of (13), stopping with the reduction of h to the number 2^{-19} (the problem was solved on a computer with 42 binary digits), we found the minimum values of the functions

$$\Phi: \Phi_I = 89.4;\ \Phi_{II} = 36.26;\ \Phi_{III} = 143.243.$$

As a result of these calculations* the final functions $a(y)$ assume the form:

$$a_I(y) = 52.37426 - 0.366222\, y_I + 0.944354 \cdot 10^{-3} y_I^2 \tag{18a}$$
$$\text{when } 37.1 \leqslant y_I \leqslant 236.2,$$

$$a_{II}(y) = 68.33766 - 0.152847\, y_{II} + 0.10721 \cdot 10^{-2} y_{II}^2 - 0.3285 \cdot 10^{-5} y_{II}^3 \tag{19a}$$
$$\text{when } 20.15 \leqslant y_{II} \leqslant 253.45,$$

$$a_{III}(y) = 52.000 - 0.3694\, y_{III} + 0.2752 \cdot 10^{-2} y_{III} - 0.8586 \cdot 10^{-5} y_{III} \tag{20a}$$
$$\text{when } 40.1 \leqslant y_{III} \leqslant 243.55.$$

It follows from analysis of the calculation results that the coefficients for the expansion of $a_I(y)$ and $a_{II}(y)$, found by the approximation method, are rather close to the values of q_λ which minimize Φ. The coefficients of the series $a_{III}(y)$ varied more significantly (the function Φ diminshed from 581.83 to 143.243), and this can be explained by the fact that the coefficients of Eq. (20) had not been accurately determined because of the presence – in the experimental curve – of a segment in which the temperature of the material underwent virtually no change.

The concluding stage of the operation is the determination of the heat-exchange coefficients for all of the above-considered cases on the basis of the following formulas:

$$\alpha_I(y) = \frac{M_I c(y)}{a_I(y) F_I}, \tag{21}$$

*The machine time for the calculation of $a(y)$ for an average-capacity digital computer is 2-5 sec; from 1 to 5 min are needed for purposes of refinement by the gradient method.

$$k_{II}(y)=\frac{M_{II}c(y)}{a_{II}(y)F_{II}}, \tag{22}$$

$$k_{III}(y)=\frac{W}{F}\ln\frac{1}{1-\frac{M_{III}c(y)}{a_{III}(y)W}}. \tag{23}$$

In these examples $c(y) = 1.83 + 0.485 \cdot 10^{-3} y$ is the heat capacity of the material in the apparatus; $M_I = 450$ kg; $M_{II} = M_{III} = 1365$ kg; $F_I = 3.0$ m^2; $F_{II} = 5.5$ m^2; $F_{III} = 8.5$ m^2; $W = 16$ kW/deg C.

The resulting relationships for the heat-exchange coefficients are shown in Fig. 3.

NOTATION

$y(\tau)$	is the temperature of the material in the apparatus, °C;
$x(\tau)$	is the temperature effect from the heat-transfer medium or from the wall of the apparatus, °C;
$a(y)$	is a continuous function of $y(\tau)$, min;
b	is a constant factor for most of the equipment, i.e., b = 1.02-1.05;
τ	is the time, min;
M	is the mass of the material, kg;
c(y)	is the heat capacity of the material, kJ/kg·deg C;
$\alpha(y)$ and k(y)	are, respectively, the heat-exchange and heat-transfer coefficients, kW/m^2·deg C;
W	is the water equivalent of one-phase heat-transfer media, kW/deg C;
F	is the heat-exchange surface, m^2;
t_S, t'_h, and t_W	are, respectively, the temperatures of the saturated vapors, of the one-phase heat-transfer medium at the inlet to the apparatus, and of the walls of the apparatus, °C.

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