DETERMINATION OF OPTIMAL CONDITIONS FOR CONVERTERS

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The necessary and sufficient conditions for optimal operation of energy and mass converters are examined, and their relations with the internal parameters-static and dynamic conductivity-are established.

The nature of numerous technological processes is determined by the laws of mass and energy transfer [1, 2].

The physical plant (apparatus) in which mass and energy transfer is accomplished, is called a converter. The limitations imposed on a given converter are determined by its finite volume, physical properties, and operating conditions. Many quite complex technological plants and processes may be represented as a certain system of energy and mass converters.

Mass and energy transfer occur as a result of the motion of various kinds of carriers interacting within the converter. The ratio of transfer flux to the gradient of forces along the transfer path is called the conductivity of the transfer path. It is convenient to distinguish between the conductivity g_1 relating to supply of energy and the conductivity g_2 relating to supply of mass. The static conductivity g = I/X is the ratio of the average values of the transfer flux I and the gradient X; the dynamic conductivity g' = dI/dX gives the increase in transfer flux with change in the gradient along the conducting path, i.e., it determines the rate of change of transfer flux. The conductivity and resistance characterize the properties of the transfer path, i.e., the internal properties of the converter. On the other hand, the conductivity may be determined from the external fluxes and forces, i.e., outside the volume of the converter. These properties of the conductivity allow it to be used as the principal parameter characterizing the operating conditions of the converter. The static and dynamic conductivities may be most simply measured at the energy input side of electrical converters.

In any transfer process motion of the carriers results in irreversible heat flow and hence converter losses. It is therefore expedient in solving this problem to invoke the theory and methods of the thermodynamics of irreversible processes [3]. Use of the Le Chatelier principle [4] allows an evaluation of the state of the system under the action of all disturbing forces, in terms of change of the internal parameters of the converter-conductivities and their functions. In analyzing the converter regimes we examine unsteady conditions at small deviations from the equilibrium state, for which a linear phenomenological law and the Onsager reciprocity relations are valid [3]. Entropy is chosen as the initial variable most fully describing the converter conditions. The statistical content of the concept of "entropy" [4] allows us to connect the phenomenological relations obtained with the statistical probability characteristics of the system.

The optimal regime of the converter is the region of conditions, consistent with the imposed constraints, under which the process proceeds at greatest intensity with minimum losses. The maximum intensity is measured by the value of the useful flux of mass and energy, and the losses by the irreversible heat flows generated in any converter. The conditions maximizing the useful flux and minimizing the irreversible heat flow, while allowing for the imposed constraints, are the criteria of the optimal converter regime.

Since the production of entropy is associated with dissipation of energy, i.e., irreversible heat flow, the state of minimum production of entropy corresponds to minimum converter losses. Prigogine [3] has shown that entropy production, which determines the outward entropy flux in any irreversible process, is a minimum in the stationary state. Hence we must seek optimal converter regimes in the region of stationary states. Realization of stationary stability is a necessary (but not sufficient) condition for the optimal regime. The optimal regime is one of a number of stable stationary states of the converter (or a combination of such states). A necessary condition for the optimal regime is minimum rate of entropy production inside the converter, which, in accordance with the extremal thermodynamic principle of [3], determines the stable stationary regime and minimum generalized converter losses.

In the optimal converter regime the absolute magitude of the sum of the products of all fluxes and forces introduced from outside is a minimum.

Let us prove this. In the stationary state – a necessary condition for the optimal regime – all the internal parameters of the converter are independent of time. This also holds true for the entropy:

$$\frac{dS}{dt} = \frac{d_e S}{dt} + \frac{d_i S}{dt}$$

For the irreversible processes under consideration $d_i S/dt$ is always greater than zero [3]. Since in the optimal regime $d_i S/dt = min$, we have

$$|d_e S/dt| = \min.$$
⁽¹⁾

According to [2],

$$\frac{d_e S}{dt} = \Delta j_S = -\frac{d_i S}{dt}; \quad j_S = \frac{1}{T} \left(\Sigma j_q - \Sigma \mu_k j_k \right). \tag{2}$$

In accordance with the Onsager theory [3], the production of entropy $\sigma = d_i S/dt$ is expressed by a linear phenomenological law-by the sum of the products of all the interacting fluxes and forces $\sigma = \sum I_i X_i$. Similarly, the rate of change of external entropy flux $d_e S/dt$, modified by the external fluxes of energy and mass (2), may be expressed by the sum of the products of the external fluxes and forces.

In fact,

$$\frac{d_{\varepsilon}S}{dt} = \frac{d}{dt} \left[\frac{1}{T} \left(\Sigma j_k - \Sigma \mu_k j_k \right) \right] = \frac{1}{T} \left(X_1 I_1 + X_2 I_2 \right),$$

where I_1 , I_2^* characterize the rates of the transfer processes [2, 3]. The thermodynamic motive force (TMF) of the energy flux X_1 is the corresponding potential gradient; for an electrical energy input this is the electric potential gradient $X_1 = \Delta \varphi$; the TMF for mass transfer is the chemical potential gradient $X_2 = -T\Delta \mu/T$.

Using (2), we have

$$\sigma = \left| \frac{1}{T} \left(X_1 I_1 + X_2 I_2 \right) \right| = \min,$$
(3)

which proves the initial proposition.

It follows that the necessary condition for the optimal converter regime may be determined from the combination of external forces and fluxes, i.e., outside the given volume. This means that information on the optimal regime of a converter may be obtained without it being necessary to penetrate inside it, however complicated the internal processes may be.

The reduction of the quality of energy introduced from outside is also characterized by ΔS_i ; this corresponds to Brillouin's negentropy ΔN_i [5]. Negentropy is produced in the plant; in accordance with the Brillouin negentropy principle [5], this is possible at the expense of conversion of information into negentropy; this information is supplied by external influences. Then the above relations also determine the quantity of information (in Shannon's sense) necessary to control the plant.

We shall now show that the input and output values and the converter parameters in the stationary regime (and for small deviations from it) may be expressed as functions of the static and dynamic conductivities along the energy channel.

We determine conditions of minimum entropy production [3]. Since σ is essentially a positive quadratic expression, the conditions for minimal σ coincide with its extreme value. This corresponds to

$$\frac{\partial \sigma}{\partial X_1} = 0; \ \frac{\partial \sigma}{\partial I_1} = 0; \ \frac{\partial \sigma}{\partial X_2} = 0; \ \frac{\partial \sigma}{\partial I_2} = 0.$$
(2a)

Introducing the notation

$$\frac{I_1}{X_1} = g_1, \frac{X_2}{X_1} = x, \frac{I_2}{X_2} = g_2, \frac{\partial I_1}{\partial X_1} = g_1', \frac{\partial X_2}{\partial X_1} = x', \frac{\partial I_2}{\partial X_2} = g_2'$$
(3a)

and making the substitution

$$\frac{\partial I_2}{\partial X_1} = g_2' x', \quad \frac{\partial I_2}{\partial I_1} = \frac{g_2' x'}{g_1'}, \quad \frac{\partial I_2}{\partial X_2} = \frac{g_1'}{x'}, \quad (4)$$

^{*}In general, we shall take as I_1 , X_1 , I_2 , X_2 any combination of external fluxes and forces, including those grouped into energy and mass fluxes. It is important that the forces and fluxes in question are intorduced into a given volume: $I_1X_1 = \Sigma I_qX_q$; $I_2X_2 = \Sigma I_kX_k$.

after substituting (3a) and (4) into (2a), we obtain

$$g'_1 + g_1 + xx'g'_2 + xx'g_2 = 0^*.$$
 (5)

Adding to (5) the Onsager relations [3]

$$I_1 = X_1 L_{11} + X_2 L_{21}, \tag{6}$$

$$L_{21} = L_{12}, (7)$$

$$I_2 = X_2 L_{22} + X_1 L_{12}, (8)$$

and taking account of (3) and (4), we obtain

$$I_1 X_1 = I_2 X_2 - g_{20} X_2^2 + g_{10} X_1^2, \tag{9}$$

$$g_1 - g_{10} = x^2 (g_2 - g_{20}), \tag{10}$$

where

$$L_{11} = \left(\frac{I_1}{X_1}\right)_{X_2=0} = g_{10}; \ L_{22} = \left(\frac{I_2}{X_2}\right)_{X_1=0} = g_{20}.$$
(11)

The quantities g_{10} and g_{20} may be determined experimentally and correspond to the initial conditions. Differentiating (9), we obtain

$$g_1 + g'_1 - xx'g'_2 - xx'g_2 - 2g_{20}xx' - 2g_{10} = 0.$$
 (12)

Solving (5) and (12) simultaneously, we obtain

$$xx' = [g_{10} - (g_1 + g_1)]/g_{20}, \tag{13}$$

$$xx' = g_{10} / [g_{20} - (g_2 + g_{20})].$$
⁽¹⁴⁾

If we supplement (13) and (14) with one of the Onsager relations, either (6) or (8), from (6) and (7) we get

$$\frac{x'}{x} = \frac{g_1' - g_{10}}{g_1 - g_{10}}, \qquad (15)$$

and from (7) and (8)

$$\frac{x'}{x} = \frac{g_2 - g_{20}}{g_2 - g_{20}} . \tag{16}$$

Equations (15) and (16) determine the relative increments of thermodynamic forces following deviations. Solving simultaneously (13) and (15), and (14) and (15), respectively, we determine the absolute values of the TMF relations and their deviations:

$$x = \pm \left[\frac{(1 - g_1^* - g_1^{'*})(1 - g_1^*)}{g_{20}^*(1 - g_1^{'*})} \right]^{\frac{1}{2}},$$
(17)

$$x' = \pm \left[\frac{(1 - g_1^* - g_1^{'*})(1 - g_1^{'*})}{g_{20}^*(1 - g_1^*)} \right]^{\frac{1}{2}},$$
(18)

where

$$g_{1}^{*} = \frac{g_{1}}{g_{10}}; g_{1}^{'*} = \frac{g_{1}^{'}}{g_{10}}; g_{20}^{*} = \frac{g_{20}}{g_{10}}.$$
 (19)

Since equations (3a) are identical, we may use one of them. Similarly, x and x' are expressed as functions of g_2 , g'_2 . Simultaneous solution of (17) and (18) and integration gives

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$$X_{1} = C \exp\left(-\frac{1}{2} \int_{t_{1}}^{t_{2}} \left\{ \left[\frac{1}{g_{1} - g_{1}} + \frac{g_{10} - g_{1}}{(g_{10} - g_{1} - g_{1})(g_{1} - g_{1})}\right] g_{1} + (20) \right\}$$

$$+ \frac{g_{1}(g_{10}-g_{1})g_{1}}{(g_{1}-g_{1})(g_{10}-g_{1})(g_{10}-g_{1}-g_{1})} + \left[\frac{g_{1}-g_{10}}{(g_{10}-g_{1}-g_{1})(g_{1}-g_{1})} + \frac{1}{g_{1}-g_{10}}\right]g_{10}\right]dt \right), \quad (20)$$
(cont^{*}d)

i.e., from the value g_1 , g_1' and their derivatives with respect to time we can measure the forces at the converter input. Similarly we determine the absolute values and the deviations of the force gradients at the converter output as functions of g_1 , g_1' and their derivatives or as functions of g_2 , g_2 , g_2 , g_2' . From (10) and (11) it is easy to determine g_2 and $I_2 = g_2X_2$. In converters involving physical and chemical conversions (chemical reactions), X_2 is the chemical affinity [3], and g_2X_2 characterizes the mass flux per unit time, i.e., the rate of physical and chemical conversion in the converter volume; g_1 and g_1' are functions of the internal properties of the plant, its physical state, geometrical dimensions, and other variable factors which change with time.

In the stationary regime – a necessary condition for the optional regime – all the parameters of the converter, including g_1 and g'_1 , are independent of time, i.e., $\dot{g}_1 = 0$; $\dot{g}'_1 = 0$. Substitution of these values into (20), (18), (17), (15), (16) shows that a necessary condition for the optimal regime is constancy of the static and dynamic conductivities along the energy (or mass) channel. Hence it also follows that to ensure a stable stationary converter regime, it is necessary and sufficient to keep constant the two quantities g_1 and g'_1 , which can conveniently be controlled without introducing information sources inside the converter.

Using the definition of the optimal regime, we shall give a quantitative estimate for it by introducing a criterion. We supplement the necessary conditions with sufficient ones, i.e., from a number of stable stationary regimes we seek the regime of maximum intensity. We introduce as criterion the quantity $p = \sigma/(|I_1X_1| + |I_2X_2|)$, which characterizes the ratio of the total losses to the sum of the useful fluxes. The optimal regime is that for which $p = \min$. Expressing p in terms of the converter parameters g_1 , g_1 , g_{10} , g_{20} , and using (10), (17), and (19), we obtain: $p(g_1^* - g_1^*)/(2-g_1^* - g_1^*)$, i.e., $p = (g_1 - g_1')/(2g_{10} - g_1 - g_1')$, or

$$p = (k_e - 1)/(k_e + 1) = \min,$$
 (21)

where

$$k_e = (g_1^{'*} - 1)/(g_1^* - 1) = \Delta g_1^{'}/\Delta g_1.$$
(21a)

The value for p may also be expressed in terms of $\gamma = I_1 X_1 / I_2 X_2$:

$$p = (\gamma + 1)/(\gamma - 1).$$
(22)



Fig. 1. Relations $p = f(k_e, \gamma)$. The region of physically possible values is shown by hatching.

From the simultaneous solution of (21) and (22) we obtain $k_e = -\gamma$. This means that when $\gamma > 0 k_e < 0$, and, conversely, when $\gamma < 0 k_e > 0$. The relations $p = f(k_e, \gamma)$ are shown in Fig. 1. It may be seen that p is the smaller, the smaller k_2 . Note that p is always greater than zero, since the generalized losses cannot be negative, while the sum of the mass and energy fluxes introduced into a given volume is always positive. Therefore condition (21) acquires the form $k_e = \min \in [1, \infty], [-1, -\infty]$.

From the expression for p for an assumed trace of σ , the signs of I_1X_1 and I_2X_2 must be opposite, i.e., $\gamma < 0$. Taking into account that p > 0, this narrows the region of possible values of $k_e: k_e \in [1, \infty]; \gamma \in [-1, -\infty]$.

The region of allowable values of k_e , γ , and p is shown by hatching in Fig. 1, and corresponds to physically realizable conditions in the converter. The condition for the optimal regime takes the form

$$k_e = \Delta g_1 / \Delta g_1, \ k_e > 1. \tag{23}$$

For variable initial conditions $k_e = \partial g_1 / \partial g_1 = \min$ and for $\gamma = g_1 / g_2 x^2 = \min$, $\gamma \in [-1, -\infty]$.

Hence a sufficient condition for an optimal converter regime is minimization of the ratio of increments of its dynamic and static conductivities. Then the necessary conditions must be met, i.e., the optimal regime is sought by making quasi-static changes in the parameters, while keeping g_1 and g'_1 constant in each regime. Criterion (23) enables the optimal regime to be determined during operation by a search method, using optimizing devices, or analytically, using variational methods. The boundary conditions describing the lower and upper limits of variation of the thermo-dynamic forces are determined by the physically attainable values of X_1 and X_2 , for which the relation

$$\frac{(I_1/X_1) - (I_1/X_1)_{X_2=0}}{(I_2/X_2) - (I_2/X_2)_{X_1=0}} = \left(\frac{X_2}{X_1}\right)^2$$
(24)

is satisfied; the latter follows from the initial equations (6)-(8). Formulation of the boundary conditions according to (24), without loss of generality, allows one to determine the working range of X_1 and X_2 on the basis of measurements of the external forces and fluxes alone. Constraints are imposed on X_1 and X_2 by the materials of which the appartus is composed and by the processed materials. The external constraints: $X_{1m} \leq X_1 \leq X_{1max}$, $X_{2m} \leq X_2 \leq X_{2max}$ and the working temperature range $\Theta_m \leq \Theta \leq \Theta_{max}$ establish the limits for I_1 , g_1 , I_2 , g_2 , g_1' , g_2' . The relations (23), (17)-(20) and their corollaries also allow one to calculate the optimal regime of the converter. This is particularly simple for electrical converters (electrothermal processes, ore-smelting furnaces, electrolytic processes, etc.).

The above approach, which allows for the close interdependence and superposition of various effects, may be applied in practice to any technological process for purposes of mathematical description and the construction of a control model. The control parameters of the model are the corresponding energy and mass fluxes, and the source of information—the static and dynamic conductivities along one of the channels. This also allows one to use the model to construct optimal control systems for technological processes.

An example of calculation of the optimal regime. We shall calculate the optimal regime and choose the basic parameters of the electrothermal process of smelting lead ore, using the experimental relation $I_1 = f(X_1)$ (Fig. 2) and initial conditions: $g_{10} \cong 1$ ohm \cdot m⁻¹ (when $X_2 = 0$) and $g_{20} \cong -0.5 \cdot 10^{-10} \text{ kg}^2/\text{sec}^2 \cdot \text{amp} \cdot \text{volt} \cdot \text{m}^3$ (when $X_1 = 0$). The dimensions are: $I_1 - \text{amp/m}^2$; $X_1 - \text{volt/m}$; $I_2 - \text{kg/m}^3 \cdot \text{sec}$ —the specific reaction rate (per unit volume); X_2 —joule/kg; $g_1 = g_1 = g_{10} - \text{ohm}^{-1} \cdot \text{m}^{-1}$; $g_2 = g_2 = g_{20} - \text{kg}^2/\text{sec}^2 \cdot \text{a} \cdot \text{b} \cdot \text{m}^3$; x-joule $\cdot \text{m/kg} \cdot \text{volt} = \text{m} \cdot \text{sec} \cdot \text{amp}/$ $kg; g_{20}^* = \frac{g_{20}}{g_{10}} - \text{kg}^2/\text{sec}^2 \cdot \text{amp}^2 \cdot \text{m}^2$. The numberical values of these quantities given below are shown without repetition of their dimensions.

Using Fig. 2 and (21a), we determine $k_{e \text{ min}}$ and find the point ε corresponding to the optimal regime; we have

 $k_{e\min} = -\gamma_{\epsilon} = 2.8; \ X_{1\epsilon} = 2.05 \cdot 10^2; \ I_{1\epsilon} = 0.39 \cdot 10^4.$

Using (17) and substituting g_1 and g'_1 corresponding to the point ε (Fig. 2), we calculate x, and then $X_2: x_{\varepsilon} = -4.4 \cdot 10^3$, whence $X_{2\varepsilon} = -0.9 \cdot 10^6$. Knowing X_2 , we choose the optimal composition of the starting raw material from those products for which the relation $I_1 = f(X_1)$ has been plotted. Here $X_{2\varepsilon} = x_{\varepsilon}X_{1\varepsilon}$.

From the formula $\gamma = I_{2\varepsilon} X_{2\varepsilon} / I_{1\varepsilon} X_{1\varepsilon}$ we find $I_{2\varepsilon}$ in terms of the known quantities γ_{ε} , $I_{1\varepsilon}$, $X_{1\varepsilon}$, $X_{2\varepsilon}$: $I_{2\varepsilon} = 0.314$. Then the main specific physical and chemical indices of the optimal process have been found.

Suppose we set ourselves a production target: Q = 1.15 kg/sec (100 ton/day), and, using the foregoing results, find the optimal volume of the plant: $V_{\varepsilon} = Q/I_{2\varepsilon}$; $V_{\varepsilon} = 3.7 \text{ m}^3$.



Fig. 2. Experimental characteristics $I_1 = f(X_1)$.

We determine the power required by the process: $P_{\varepsilon} = I_{1\varepsilon}X_{1\varepsilon}V_{\varepsilon}$; $P_{\varepsilon} = 2.96 \cdot 10^3$ kwatt.

We determine the optimal geometry of the proposed plant: furnace height H; furnace area S; electrode diameter d. For this we use the following equations: a) SH = V; b $\frac{I_1}{X_1} = \frac{S}{H} = G$; where G is the furnace conductivity determined as a function of the electrode depth h_e from the formula $G = \frac{3\pi dg_1}{\ln(4H/d)}$ for $(h_e/H)_e = 0.5$ [7]; hence b) $\frac{S}{H} = 3\pi d/\ln(4H/d)$. The relation between the electrode diameter and the reduced furnace diameter D is determined on the basis of the known current density in the electrode I_{1e} and in the furnace: $I_{1e}/I_{1e} = D^2/d^2$, assuming $I_{1e} = 6 \cdot 10^4$ for graphite electrodes. We obtain the equation c) $(D/d)_e^2 = 3.46$; where $D = \sqrt{4S/\pi}$. By simultaneous solution of a), b), and c) in the unknowns H, d, and S, we determine their optimal values:

$$H_{\varepsilon} = 1.23 \text{ m}; d_{\varepsilon} \cong 1 \text{ m}; S_{\varepsilon} = 2.95 \text{ m}^2.$$

Assuming, for simplicity, that the furnace is single-phase, we find the optimal electrical parameters: current I^{U} and voltage U:

$$I_{z}^{0} = I_{1z} \frac{\pi d^{2}}{4}; \ I_{z}^{0} = 47 \cdot 10^{3} \text{ amp}$$

The furnace phase voltage $U_{\varepsilon} = p_{\varepsilon}/I_{\varepsilon}^{0}$; $U_{\varepsilon} = 63$ volts. We also choose the furnace transformer.

Industrial ore-smelting furnaces have parameters very close to those obtained.

In an automatic process control system the point ε is determined by computers and an optimization system. In this case perturbing forces deflect the course of the process.

NOTATION:

 g_1 , g_1 -static and dynamic conductivities of the converter with respect to supply of energy; g_2 , g_2 -the same with respect to supply of mass; X_1 , X_2 -sums of the external thermodynamic forces determining, respectively, the flux of energy (I₁) and of mass (I₂); I_q , X_q -individual energy fluxes and corresponding thermodynamic forces; I_k , X_k -individual mass fluxes and corresponding forces; j_q -total energy flux; $\Sigma \mu_k j_k$ -total mass flux; μ_k -mass transfer potential; ϕ -electrical potential; j_k -mass flux; j_s -external entropy flux; d_eS/dt -rate of influx of entropy from outside; d_iS/dt -rate of growth of entropy ΔS_i inside system as a result of irreversible processes; for a real process Td_iS/dt expresses energy dissipation per unit time; continuity of the process is ensured by compensation of losses by the influx of entropy from outside ΔS_e ; T-absolute temperature; x-coefficient representing ratio of total thermodynamic forces; g_{10} , g_{20} -initial values of g_1 and g_2 , respectively, for $X_2 = 0$, $X_1 = 0$; p-specific generalized loss coefficient; k_e -optimality criterion expressed as ratio of increments of energy conductivities; γ -specific coefficient of energy converter; Q-output; P-power; S-area; H-height of furnace; V-volume; G-total conductivity of furnace for electrode depth h_e ; d-electrode diameter; I_{1e} , X_{1e} , X_{2e} , I_e^0 , U_e , etc.-corresponding optimal values of the parameters.

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