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Thermodynamic Modeling on Graphs

Formulas are written figures.

Figures are drawn formulas.

D. Hilbert

3.1. Problem Statement and History

The question on the effectiveness of geometrical methods for development and interpretation of extreme thermodynamic models is evidently subject to essential subjectivism and partiality. So, whereas Newton in his *Principles* started to solve each of more than 200 considered problems with graphical explanations, and only then passed to formulas, Lagrange in *Mechanique Analytique* did not present any drawings, demonstrating thus the possibility of constructing the “building” of mechanics without graphical representation.

Though in thermodynamics, geometrical methods have been applied starting with Gibbs’s classical works, in the works known to the authors on computer modeling of thermodynamic systems, such methods have not been practically used. Our reference to graphical construction is based on the assumption that graphs should provide an insight into mathematical peculiarities of the problems solved, on the one hand, and contribute to expansion of the sphere for applications of extreme models, on the other.

Yet Kirchhoff had shown the possibility of reducing problems dealing with the study on multidimensional systems to problems on graphs. In [111] he tested the revealed theoretical relationships for current and potential distribution in the flat round plate by comparison with the experimental results on the electric circuit, i.e., on the object with the scheme in a graph form. Thus, he established the correspondence between electric fields in the continuous two-dimensional space and on the one-dimensional continuum, i.e., the “graph.” Kirchhoff deduced his known laws of current distribution for graphs and showed in [112] how to derive an independent system of equations by using these laws, choosing the calculated

loops corresponding to chords, that is, edges that remain after separation of the spanning tree from the closed graph.

In later works on the theory of electric circuits [108–110] Kirchhoff factually constructed a complete system of models to study these circuits. In [108] he showed the possibility of a transition from solving a closed system of equations (of Kirchhoff's laws) to the extreme problem – the search for the minimum heat generation in a passive circuit (one without sources of electromotive forces). To put it differently, he suggested an extreme model of current distribution. In [109, 110] the motion equation (the Ohm law) is derived in terms of the equilibrium of forces acting on “electric liquids,” and the considered equilibrium in this case can be interpreted as the thermodynamic one.

Kirchhoff's works make clear the possibility of equivalent mutual transformations of models that are based on different physical principles (conservation, equilibrium, extremality); Kirchhoff's analysis also substantiates the transition from such models, including extreme thermodynamic multidimensional systems, to graphical models.

Maxwell suggested the *method of potentials* [129] for calculation of electrical circuits as graphs, which is equivalent to the method of loop currents based on Kirchhoff's circuit laws of conservation. At about the same time Gibbs introduced in the thermodynamics the method of potentials for multidimensional continua [53].

Geometrical methods were developed by A. N. Gorban in *Equilibrium Encircling* for thermodynamic analysis of chemical system kinetics. These methods made it possible for one to pass from searching the extremum of the Lyapunov thermodynamic function on the material balance polyhedron to searching for it on the graph called a *thermodynamic tree*. This tree vividly and simply represents an aggregate of paths along which the Lyapunov function changes monotonically and the sets of compositions attainable from the initial state of a system (*the thermodynamic attainability region*). It is constructed by the relations of thermodynamic equivalence of x_1 and x_2 : That is, $x_1 \sim x_2$ if there exists a continuous curve running from the composition x_1 to the composition x_2 along which the thermodynamic Lyapunov function is constant. Identification of thermodynamically equivalent compositions with respect to each other enables transformation of the domain of definition of the studied function to one-dimensional space, namely the tree, which facilitates substantially the analysis of processes in chemical systems.

Studies similar to those performed by A.N. Gorban, but belonging to pure mathematics were conducted by A.S. Kronrod [116] and V.I. Arnold [10]. Their works were aimed at solving the thirteenth Hilbert problem, i.e., representation of the continuous function of many variables as a superposition of continuous functions of a lesser number of variables [69]. A.S. Kronrod suggested a method to transform a multidimensional domain of definition of functions into a one-dimensional continuum, the *tree of functions* (which can be handled as the mathematical generalization of the notion of the thermodynamic tree); V.I. Arnold applied such a tree to obtain exact and approximate representations of some specific functions.

In our opinion the idea of a tree is interesting from the general principles of mathematical programming (MP)—the principles for solving extreme problems. Actually each MP method is characterized by the rule that determines at each step of the computational process a direction of motion and a path length over the function surface whose extremum is sought for. If we use the tree with set initial state and convexity of considered function, our choice of trajectory becomes unambiguous.

Note also the paper by A.I. Volpert [168], in which *bichromatic* graphs are applied to the qualitative analysis of solutions to differential equations of definite form for the problems of chemical kinetics. The work [28] presents a rather wide view of the application of topology and theory of graphs to quantum chemistry.

B.M. Kaganovich employed extreme thermodynamic models to study hydraulic circuits [77–79], i.e., objects whose structure is naturally represented as graphs. In so doing, he proceeded from the concepts of the *hydraulic circuit theory* (HCT), which was founded by V.Ya. Khasilev and A.P. Merenkov [104–107, 132, 130].

Creation of extreme thermodynamic models of flow distribution in circuits and physical interpretation of HCT on their basis provided a deeper insight into this theory, facilitated correct comparison of its methods, and enhanced potential of its applications. Thus, the low sensitivity of extreme methods to change in the space of variables made a wide variation of problem statements possible, e.g., inclusion of diverse constraints on parameter regulation in the models of post-emergency regimes of pipeline networks. The ideas of thermodynamic modeling of hydraulic systems may turn out to be useful in studying electric networks as well.

As a result of the thermodynamic analysis of HCT the problem of modeling heterogeneous hydraulic circuits (i.e., circuits with multiphase chemically reacting flows in the branches, or graph arcs) was formulated in [91]. Studies of this problem substantially extended an area of HCT applications.

B.M. Kaganovich also made attempts to employ jointly thermodynamics and the hydraulic circuit theory to analyze multidimensional continua. The works [81, 83, 85] interpret *model of extreme intermediate states* (MEIS) with the variable ξ in the graphical form and represent some other extreme models of chemical systems with the specified mechanism of reactions in the form of hydraulic systems. In [91] MEIS of spatially inhomogeneous structures, which is somewhat different than the model of (2.97)–(2.105), is interpreted as a hydraulic circuit to study atmospheric pollution processes.

Descriptions of continua in the form of circuits certainly make sense, if for no other reason than the joint analysis of several possible mathematical models of one and the same object contributes to deeper understanding of it's the object's physical properties. On the whole, graphical models are useful in substantiating applicability of thermodynamics concepts to different types of physicochemical systems. If we manage to represent the studied function as a function of no more than two variables for each graph branch, then because of the holonomy of the corresponding Pfaffian forms it becomes possible to prove its possible representation as a differentiable potential function, which determines applicability of thermodynamics techniques.

Below we discuss just two, seemingly most topical, “graphical” ideas: a thermodynamic tree proposed by A.N. Gorban and thermodynamic modeling of multiloop hydraulic systems.

3.2. Thermodynamic Tree

The effectiveness of the idea of a thermodynamic tree, which was called in [58] an “entropy tree,” will be illustrated at first by our “through” example of hexane isomerization. Fig. 3.1*a* presents the same triangle of the material balance as Fig. 2.4*a*, but with some additional details. Different kinds of hatching are used to denote five components of the *arcwise connectedness*. These are regions in each

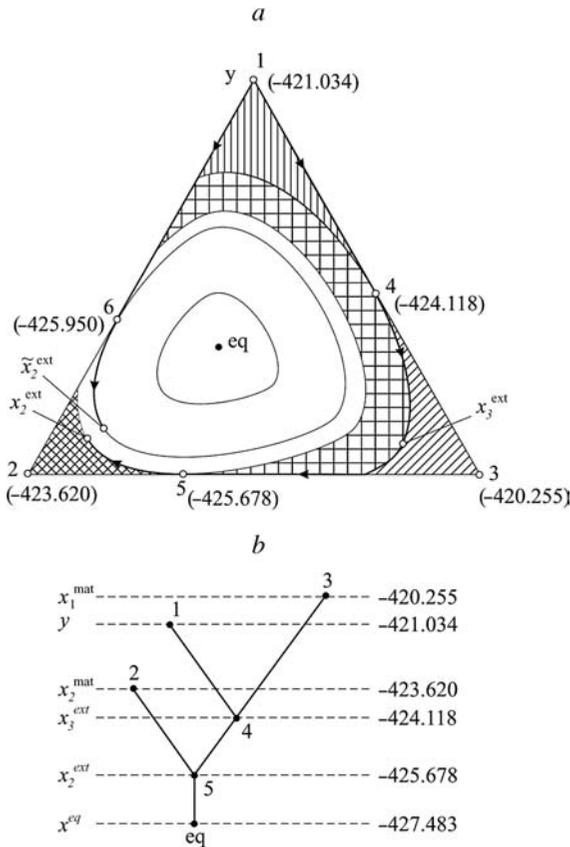


FIGURE 3.1. Polyhedron of material balance (a) and the thermodynamic tree (b) for the hexane isomerization reaction, $T = 600$ K, $P = 0.1$ MPa.

of which any two points can be connected by a thermodynamically admissible path.

Fig. 3.1*b* shows the thermodynamic tree whose branches have a one-to-one correspondence with the regions hatched in Fig. 3.1*a*. Every point of the tree represents an intercept of a line $G = \text{const}$ belonging to the corresponding component of connectedness. The points on this intercept satisfy the linear balance:

$$\sum_j G_j x_j = G = \text{const.} \quad (3.1)$$

The constructed tree that replaces the polyhedron $D(y)$ allows the study on the behavior of the Gibbs energy (a thermodynamic Lyapunov function in this case) and the objective function (2.38). Suppose that the initial state y is represented by the vertex 1 ($y = (1, 0, 0)^T$) and the process objective is to obtain a maximum possible quantity of the isomer x_3 (the objective function (2.38) takes the form $F(x) = x_3$). The desired maximum point on $D(y)$ is obviously vertex 3. We can move to it from y along tree branch 1–4, monotonically decreasing the function $G(x)$. However, after point 4 is reached, further movement to 3 becomes impossible because the Gibbs energy monotonically increases on branch 3–4 from 4 towards 3. Point 4 determines a level of G (the isopotential surface of $G = -424.118$ kJ/mole), at which the extreme composition x_3^{ext} (the linear function maximum is achieved at the convex set boundary) should lie.

With the choice of vertex 2 as an initial state y and the new maximization of x_3 , the solution will be on the surface $G_5 = -425.678$ kJ/mole. When we maximize x_2 the same Gibbs energy level is attained from the initial states 1 and 3.

Note that when we solve all the mentioned problems:

$$\begin{aligned} y &= (1, 0, 0)^T, & \max x_3, \\ y &= (0, 1, 0)^T, & \max x_3, \\ y &= (1, 0, 0)^T, & \max x_2, \\ y &= (0, 0, 1)^T, & \max x_2, \end{aligned}$$

there is a situation of the “thermodynamic pothole,” for which we cannot indicate the exact Gibbs energy levels $G(x^{\text{ext}})$ (see Section 2.4). Application of the tree overcomes the difficulty that arises. Fig. 3.1*a* illustrates a potential benefit thanks to improvement of the obtained problem solution by the thermodynamic tree. If we moved from vertex 1 to vertex 2 (tending to $\max x_2$), reached the point $\min G$ on the intercept 1–2 (point 6) and then continued to move along the curve $G = G_6$, we would be able to reach the point \tilde{x}_2^{ext} , which contains the component x_2 in a somewhat lesser amount than at the point of exact solution x_2^{ext} (the errors of different algorithms are discussed in Chapter 4).

The tree can be applied to the analysis of situations, when the stated problem’s solution proves to be degenerate. For hexane isomerization such a situation occurs at maximization of the total amount of any two components and at equality of each coefficient c_j in (2.38) to unity (see Section 2.4). If we find, for example, $\max(x_2 + x_3)$ and $y = (1, 0, 0)^T$, all the points of edge 2–3 (Fig. 3.1*a*) belonging

to $D_t(y)$ are the points of the objective function maximum. This situation can be analyzed using the tree on the natural assumption that we are equally satisfied with two extreme cases: 1) $x_2 = 1, x_3 = 0$; and 2) $x_2 = 0, x_3 = 1$, and hence we may try to reach vertices 2 and 3. In the first case the sought Gibbs energy level will be $G = G_5$ and in the second, $G = G_4$. In Fig. 3.1a the region of extreme solutions that is part of edge 2–3 and lies between the point of its intersection with the curve $G = G_4$ and the point of contact with the curve $G = G_5$ corresponds to the determined range of levels $G_4 - G_5$. In Fig. 3.1b the range of possible solutions is represented by branch 4–5 of the tree.

When some arbitrary point of the triangle edge or the internal region rather than its vertex corresponds to the initial composition, we start moving on the tree not from one of the vertices, but from the internal point of a branch corresponding to the initial Gibbs energy level and the initial component of arcwise connectedness.

The idea of the thermodynamic tree is further discussed based on Fig. 3.2a and b, taken from *Equilibrium Encircling*. There, this idea was illustrated on the example of hydrogen combustion in oxygen. The vector x comprised in that case six components: H_2, O_2, H_2O, H, O, OH , and two components of the vector y are taken as: $y_{H_2} = 2$ and $y_{O_2} = 1$. Fig. 3.2a presents the graph \tilde{D} of the balance polyhedron $D(y)$ and Fig. 3.2b presents the thermodynamic tree.

Assume that we maximize the amount of water (x_{H_2O}) achievable from the vertex H_2, O_2 as the initial state. According to the material balance conditions, the maximum admissible concentration of water corresponds to the vertex H_2O . From Fig. 3.2 it is easy to see that for the analysis of the properties of the problem we require not the whole tree (13 branches and 14 vertices), but only a smaller part of it (4 branches and 5 vertices). This smaller part is indicated in Fig. 3.2 by bold lines. Hence, in some cases it is possible in principle to reduce graphical constructions to solve specific problems. One should certainly remember that the

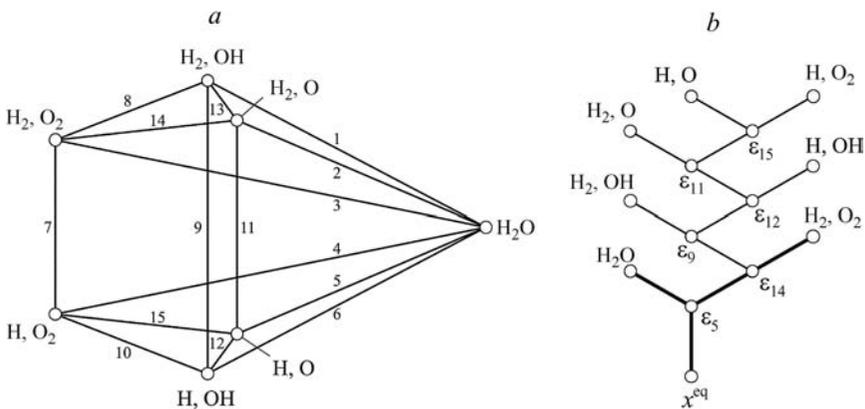


FIGURE 3.2. A graph of the polyhedron of material balance (a) and thermodynamic tree (b) for the reaction of hydrogen burning.

TABLE 3.1. Combinations of C_m^n

m	n			
	20	50	100	200
3	1140	$1.96 \cdot 10^4$	$1.62 \cdot 10^5$	$1.31 \cdot 10^6$
5	$1.55 \cdot 10^4$	$2.12 \cdot 10^6$	$7.53 \cdot 10^7$	$2.54 \cdot 10^9$
10	$1.89 \cdot 10^5$	$1.03 \cdot 10^{10}$	$1.73 \cdot 10^{13}$	$2.25 \cdot 10^{16}$
20	1	$4.71 \cdot 10^{13}$	$5.36 \cdot 10^{20}$	$1.61 \cdot 10^{27}$

only thing left to do is to develop algorithms that would allow the researcher to construct a needed part of the tree.

The algorithm described in [58] supposes that the graph \tilde{D} of the whole polyhedron is known. However, in studies of real systems the polyhedron (and, thus, the graph) can reach astronomical sizes because the maximum possible number of vertices of $D(y)$ corresponding to the system of m linear equalities with n unknowns is determined by the formula

$$C_m^n = \frac{n!}{m!(n-m)!}.$$

The swift growth of this number with increasing dimensionality of the problem is illustrated in Table 3.1.

The above two examples show that it is possible for the number of elements (vertices or branches) of the tree to exceed considerably the number of elements in $\tilde{D}(y)$.

We can reduce the dimensionality of thermodynamic trees by two approaches. In the first we decrease dimensionality of the vector x . Its application is admissible in cases where several macrocomponents, whose concentrations are by many orders of magnitude higher than the concentrations of other components in the reacting mixture, can be isolated in chemical systems. It is clear that these components determine, with an inessential error, a surface shape of the thermodynamic function corresponding to the problem solved. If x is chosen properly, inclusion of a small number of the sought microcomponents in the list of the components of x can lead to addition of the admissible (in terms of calculations) number of “microbranches” to the “macrotree.” System components are divided into micro and macro rather easily when the thermodynamic analysis is applied to environmental problems involving the search for quantities of substances that can be dangerous, for example, at concentrations of 10^{-10} – 10^{-12} of the total system.

The second approach consists in construction of the tree equivalent not to the whole balance polyhedron but to only one face of special interest for the researcher. In the analysis of environmental characteristics of combustion processes it may be interesting to reveal interrelations between formations of nitrogen oxides and carbon monoxide. This problem can be properly analyzed if we use the face whose vertices correspond to the maximum concentrations of NO_x and CO in terms of the material balance, and the point y . Mathematically this approach

is equivalent to the first one, since the polyhedron face can be treated as a polyhedron corresponding to the reduced dimensionality of the space of variables. When we construct flat two-dimensional faces, an approach that is convenient from the standpoint of graphical interpretation of the problem solved, in order to choose a list of the vector x components, we should apparently apply the relation

$$n = m + 2,$$

where n is the dimensionality of x , and m is the number of linear material balances.

With the efficient application of both approaches the algorithm presented in [58] may also be admissible in terms of calculation time. Of course, it does not mean that the search for new effective algorithms for constructing thermodynamic trees is not advisable. Irrespective of the success in these efforts the theoretical value of the “idea of tree” is unquestioned. A sketch variant of the algorithm of tree construction on the basis of the second approach is discussed in Section 4.4.

3.3. Thermodynamic Interpretations of Hydraulic Circuit Theory

Historical Background

Relations between thermodynamics and hydrodynamics, and hence hydraulic circuit theory, since the latter can be handled as part of the hydrodynamics from the standpoint of physics, were considered in Section 1.3.

The methods of *loop flows* (currents) and *nodal pressures* (potentials) are known to be basic in describing flow (current) distribution. In so far as they are analogs of the methods of cycles and potentials in the thermodynamics, they emerged almost simultaneously with the latter (the methods of cycles and loop currents are suggested by Clausius and Kirchhoff; the methods of potentials in the thermodynamics and the circuit theory are suggested by Gibbs and Maxwell). Kirchhoff [108] and Maxwell [129] who are the founders of the theory of electric circuits, showed the possibility for transition from their methods to extreme models. In [129] Maxwell also established mathematical equivalence of the methods of potentials and loop currents.

Both the method of loop currents, whose mathematical prerequisite is the equality to zero of the integral over a closed loop, and the method of potentials are only applicable to studying equilibrium systems that can be defined as “conservative” ($\oint df = 0$) and as “potential” (see Chapter 1). Note that Euler was the first to introduce, in 1765, the potential function into hydrodynamics and physics as a whole.

Section 1.3 of the book has already presented equilibrium interpretations of the laws of motion of electric charges (Ohm’s law) and viscous liquid (the Darcy–Weisbach law). In addition we recall here an equilibrium nature of the classical

system of hydrodynamics equations:

$$\frac{\partial \rho}{\partial \tau} + \operatorname{div}(\rho w) = 0, \quad (3.2)$$

$$\rho \frac{dw}{dt} = \rho F - \nabla P + (\eta + \zeta) \nabla \operatorname{div} w + \eta \Delta w, \quad (3.3)$$

$$\begin{aligned} c_p \rho \frac{dT}{d\tau} - \frac{dP}{d\tau} = & q + \operatorname{div}(\chi \nabla T) \\ & + \left\{ \zeta (\operatorname{div} w)^2 + 2\eta \left[\left(\frac{\partial w_x}{\partial x} \right)^2 + \left(\frac{\partial w_y}{\partial y} \right)^2 + \left(\frac{\partial w_z}{\partial z} \right)^2 \right] \right. \\ & \left. + \eta \left[\left(\frac{\partial w_x}{\partial y} + \frac{\partial w_y}{\partial x} \right)^2 + \left(\frac{\partial w_x}{\partial z} + \frac{\partial w_z}{\partial x} \right)^2 + \left(\frac{\partial w_y}{\partial z} + \frac{\partial w_z}{\partial y} \right)^2 \right] \right\}, \end{aligned} \quad (3.4)$$

$$P = f_1(\rho, T), \quad S = f_2(\rho, T), \quad (3.5)$$

where ρ is density; τ is time; w is velocity; F is volumetric force; η , ζ are coefficients of dynamic and volumetric viscosity; c_p is specific heat capacity at constant pressure; q is the heat quantity supplied to a unit volume in a unit time due to nonmechanical reasons; and χ is a coefficient of thermal conductivity.

Equation (3.2) describes a flow continuity condition. The Navier-Stokes equation (3.3) is an extension of Newton's second law to moving liquid. Equation (3.4) formulates the energy conservation law. Relations (3.5) are the thermal and caloric state equations, respectively. Inclusion of the state equations into system (3.2)–(3.5) implies application of the assumption on the equilibrium thermodynamic nature of liquids dynamics.

In the 1960s V.Ya. Khasilev extended the main statements of electric circuits theory developed in late 19th century, applying them to multiloop hydraulic circuits. The equilibrium nature of the liquid flow equations proves the validity of such an extension. In the basic works on hydraulic circuit theory [104–107, 132, 130] V.Ya. Khasilev made a comparative analysis of computational properties for the methods of loop flow rates and nodal pressures, and he suggested extreme methods (MP) for solving HCT problems. He outlined thereby two directions in MP application: 1) calculations of flow distribution and 2) technical and economic optimization of hydraulic networks. In the first case the objective function form was determined from the Kirchhoff-Maxwell heat theorem on least heat production in a passive circuit [130].

V.Ya. Khasilev showed the impact of *closing relations* (relations between the pressure losses and the flow rates in circuit branches) on mathematical features of the optimization problems of circuit schemes and parameters (namely, convexity or concavity of the objective function and its slight slope near the extremum point) [104, 106]. In their book, A.P. Merenkov and V.Ya. Khasilev [130] studied these relations mainly in terms of the accuracy of flow distribution calculations.

A.P. Merenkov and N.N. Novitsky performed a rather detailed analysis of the inverse flow distribution problems [132, 130, 134].

O.A. Balyshev extended the HCT principles to the analysis of nonstationary flow distribution in networks [16–18]. From the joint solution of the equations of continuity, Navier–Stokes, and state, he obtained formulas of closing relations for motion of media with constant density and media subject to the equation of state for the ideal gas (or real gas with constant compressibility).

B.M. Kaganovich formulated the problems of thermodynamic interpretation of HCT and study of heterogeneous hydraulic circuits, i.e., circuits with a complex phase and chemical composition of flows [85, 91].

Fundamentals of Hydraulic Circuit Theory

The cited work [130] presents two definitions of hydraulic circuits (HCs). According to the first definition, HCs represent an aggregate of conductors intended for transportation of liquids. The second defines HC as a mathematical model consisting of two constituents: a calculated scheme in the form of the directed graph [180]; and algebraic relations describing flow of liquids (gases) along graph's arcs. The present book applies only the second definition as the most adequate to its purposes.

HCT studies direct and inverse problems of flow distribution in hydraulic circuits and problems of the *optimal synthesis* (choice of the schemes and parameters) of circuits. The latter are usually related to the technical and economic optimization of pipeline networks (water, heat, oil and gas supply, etc.).

For real objects HCT has studied three key types of models up to now:

- 1) circuits with lumped parameters, in which the resistances of branches (graph arcs) and effective heads are independent of flow distribution;
- 2) circuits with variable (regulated) parameters, in which at least part of the branch characteristics (effective heads, heads and sinks (sources) at nodes, etc.) are the functions of sought quantities, and determined (“regulated”) by the flow distribution itself;
- 3) circuits with distributed parameters, in which the characteristics of branches (resistances, effective heads) alter depending on distances to the nodes adjacent to the corresponding branch.

If all relationships for the branches of a distributed or regulated circuit are represented as a differentiable function of no more than two variables (for example, length and time or length and temperature), then the closing relations for them may be written in a “lumped” integral form, at least theoretically. At the same time the holonomy of the Pfaffian forms makes the thermodynamic representation of hydrodynamic relationships feasible.

For each mentioned model, the circuit branches are divided into active (with sources of effective heads: pumps, compressors, gravity, wind pressure, etc.) and *passive* (without such sources). By the graph theory the circuit scheme (part of the

scheme) without closed loops is called a *tree* and the branches supplementing the tree to the closed (cyclic) scheme are called *chords*.

Application of the thermodynamics concepts in HCT calls for expansion of the accepted classifications of models and the system of notions. Open and closed, homogeneous and heterogeneous circuits naturally supplement the classification. The open circuits have sources and sinks: As do any other open thermodynamic systems, they exchange substance with the environment. In the closed circuits sources and sinks are absent.

There are two approaches to division of hydraulic circuits into *homogeneous* (uniform) and *heterogeneous* (nonuniform) types. In thermodynamics the heterogeneous systems include those in which a substance is present in different phases. Based on thermodynamic terminology we can assume conditionally that the flows in different circuit branches subject to different closing relations (e.g., flows corresponding to turbulent and laminar flow modes) belong to different phases. Therefore, the circuits with the distinct relationships between head losses and flows in the branches can be considered heterogeneous. This classification of circuits was suggested in [81].

In this context, the book addresses basically heterogeneous circuits, ones in which flows in separate branches contain several phases. In general, such flows are the vectors whose components are the flows of different chemical substances in different phase states on the branch.

For circuits with lumped parameters the problems of stationary flow distribution calculation are described in [130] in three ways: a) on the basis of the loop system of equations; b) using nodal potentials; c) in the extreme statement on the basis of the minimum heat production theorem.

The loop system of equations has the form:

$$Ax = Q, \quad (3.6)$$

$$Bh = BH, \quad (3.7)$$

$$h_i = f_i(x_i), i = 1, \dots, n, \quad (3.8)$$

where x and x_i are a vector of flows in the circuit branches and its i th component, respectively; $A = [a_{ij}]$ is an $(m - 1) \times n$ -matrix of connections of independent nodes to branches; $a_{ij} = 1$, if the flow in the i th branch runs to the j th node in accordance with the specified direction; $a_{ij} = -1$, if the i th flow runs from the j th node and $a_{ij} = 0$ if j does not belong to branch i ; Q is a vector of external sources and sinks at the nodes

$$\sum_{i=1}^m Q_j = 0;$$

m is the number of nodes; n is the number of branches; h and h_i are a vector of head losses and its i th component, respectively; H is a vector of effective heads; $B = [b_{ki}]$ is an $c \times n$ -matrix of the coincidences of loops and branches; $b_{ij} = 1$ if the initially specified direction of flow in the branch coincides with the specified

direction of loop encircling; $b_{ij} = -1$ when these directions are opposite; $b_{ij} = 0$ when the i th branch is not included in loop k .

The matrix equation (3.6) describes the first Kirchhoff law, which expresses the requirement of mass conservation in the flows of liquid for hydraulic circuits. Equation (3.7) formulates the second Kirchhoff law, which may be interpreted as the extension of the general energy conservation principle to separate circuit loops. Expression (3.8) is a closing relation.

For the method of nodal potentials equation (3.7) in system (3.6)–(3.8) is substituted by the equation

$$h - H = \bar{A}^T \bar{P}, \tag{3.9}$$

where $\bar{A}^T = [a_{ij}]$ is an $m \times n$ complete transposed matrix of connections of nodes to branches; \bar{P} is a vector of nodal pressures.

The extreme principle of flow distribution in circuits as based on the works by Kirchhoff and Maxwell is formulated in [130] as the *heat theorem*. It means that flows in the open passive circuit are distributed so that they produce a minimum amount of heat. The corresponding mathematical problem is formulated in this case as the following:

Find

$$\min \sum_i h_i x_i \tag{3.10}$$

subject to

$$\begin{aligned} Ax &= Q, \\ h_i &= f_i(x_i), i = 1, \dots, n. \end{aligned}$$

The authors of [130] also studied the possible extension of the theorem about least thermal effect on active circuits, in particular with different exponents β in the closing relations (see below). This was done by such variation of the objective function type that the solution to the extreme problem coincided with the solution to the system of equations (3.6)–(3.8). As a result the following function was determined:

$$F(x) = \sum_{i=1}^n \left(\frac{f_i(x_i)x_i}{1 + \beta} - H_i x_i \right). \tag{3.11}$$

In [78] it is shown that this formula can be derived directly from the Lagrange principle of virtual work. Actually for hydraulic circuits this principle is interpreted as follows. If the flow distribution in the circuit is equilibrium, i.e., the equilibrium of all forces exerted on a moving medium (pressure, friction, gravity, etc.) is observed in every section of every branch, the work done on any infinitesimal deviation of flows in the branches from their equilibrium values equals zero. Mathematically, this principle is interpreted as follows:

$$dL = z_i x_i^\beta dx_i - H_i dx_i = 0, i = 1, \dots, n, \tag{3.12}$$

where z_i is the resistance of the i th branch.

Obviously equation (3.12) represents an extremum condition of the objective function (3.11) and reveals its physical sense. $F(x)$ is the variation of energy of the total flow in the circuit at its deviation from the optimal (equilibrium) value (the Lagrange function). It is clear that the principle of virtual work allows an easy determination of the extremality criterion for passive circuits ($H = 0$).

The closing relations $f_i(x_i)$ for incompressible liquids for the HCT problems in [92] are represented in two forms:

$$h_i = f_i(x_i) = z_i x_i^\beta, \quad (3.13)$$

$$h_i = z_{i1} x_i + z_{i2} x_i^2. \quad (3.14)$$

These relations can be applied to model characteristics of the sources of effective heads by the equation

$$H = H^0 - z_{\text{in}} x_{\text{in}}^\beta, \quad (3.15)$$

in which the second term on the right-hand side is a head loss in an imaginary branch simulating the internal resistance of a pump.

The formulas to determine z from the Darcy–Weisbach equation and experimental relations for the friction coefficient λ were studied in [132] from the computational standpoint.

V.Ya. Khasilev [104, 106] and, later, B.M. Kaganovich [76] examined the effect of type of closing relations on the mathematical properties of problems pertaining to technical and economic optimization of hydraulic circuits. V.Ya. Khasilev performed the analysis on the basis of the following formula of pipeline diameter that was derived from the elementary transformation of the Darcy–Weisbach equation

$$d = a x^\psi h^{-\varphi},$$

Where a , ψ and φ are coefficients. For turbulent flow ($\beta = 2$) $\psi \approx 0.38$ and $\varphi \approx 0.19$.

Assume, for an objective function that indicates some cost characteristic of the network, that the function's term are proportional to d_i in the problem of technical and economic optimization; in the case of $1 \leq \beta \leq 2$ this function proves to be convex by the axes h_i and concave by x_i . In the extremum point h here it will be characterized by the exceptionally slight slope (the small curvature). The doubling of head loss in comparison to optimal value increases the liquid transportation cost by 4.6%, and a twofold decrease in the loss leads to just a 3.8% cost increase. Some adjustments in the results of analysis made by V.Ya. Khasilev were performed in [76] in terms of constraints on the conditions of network development and upgrading.

The methods of network optimization and solutions to direct and inverse problems of flow distribution that were developed in HCT are presented in detail in [130]. On the whole, hydraulic circuit theory has been applied extensively for several decades to solve engineering problems of development and operation of pipeline, and of other hydraulic networks with flows homogeneous in their chemical and phase compositions.

Models of Nonstationary Flow Distribution

O.A. Balyshev extended HCT principles to the analysis of nonstationary flow distribution in multiloop hydraulic systems using the premises of the “equilibrium dynamics” [16–18]. In the context of our discussion his results are of interest as the basis for thermodynamic studies on nonstationary processes in complex hydraulic networks. Application of the thermodynamic analysis to the hydraulic shock in a separate pipe was demonstrated in Section 1.3.

The laws of mass and energy conservation, as is customary in HCT, were written by O.A. Balyshev in the circuit (Kirchhoff) form, and closing relation type was determined by transforming the Navier–Stokes and state equations.

For the circuits with lumped parameters, O.A. Balyshev’s model has the form

$$Ax(\tau) = Q(\tau), \tag{3.17}$$

$$Bh(\tau) = BH(\tau), \tag{3.18}$$

$$h_i = f_i(x_i(\tau)), \quad i = 1, \dots, n. \tag{3.19}$$

In the simplest case, when each i th flow of incompressible liquid experiences only forces of inertia, pressure and friction, the form of the functions f_i is determined from the initial Navier–Stokes equation

$$\rho \frac{dw}{d\tau} = -\frac{dP}{dl} - \lambda \frac{\rho w^2}{2d}, \tag{3.20}$$

or from

$$\frac{dx(\tau)}{d\tau} = -\frac{\pi d^2}{4} \frac{dP}{dl} - \frac{2\lambda x^2(\tau)}{\pi d^3 \rho} \tag{3.21}$$

when we pass from velocity w to mass flow x .

From here we have the differential closing relation

$$-dP = \frac{8\lambda x^2(\tau)}{\pi^2 d^5 \rho} dl + \frac{4}{\pi d^2} \frac{dx(\tau)}{d\tau} dl. \tag{3.22}$$

Introduction of the notion of instantaneous head (pressure) drop

$$h_i = P_i(0, \tau) - P_i(l_i, \tau), \tag{3.23}$$

will lead to

$$h_i = \frac{8\lambda x_i^2(\tau)}{\pi^2 d^5 \rho} l + \frac{4}{\pi d^2} \frac{dx_i(\tau)}{d\tau} l \tag{3.24}$$

or

$$h_i(\tau) = f_i(x_i(\tau)) = z_{i1} x_i^2(\tau) + z_{i2} \frac{dx_i(\tau)}{d\tau}. \tag{3.25}$$

Model (3.17)–(3.19) enriched the hydraulic circuit theory in terms of opportunities it afforded to analysis of network stability to variations in the vectors H , Q and Z , and to optimization of operation conditions.

Thermodynamic Models

We seek to determine a type of the objective function for an extreme thermodynamic flow distribution model for a closed active circuit with lumped parameters and isothermal liquid flow. In such a function the entropy production in the i th branch will be represented by the relation

$$\Delta S_i = \Delta q_i T^{-1} = h_i x_i T^{-1}, \quad (3.26)$$

which is based on the assumption on the equalities

$$T_i = T_{\text{env}} = T, i = 1, \dots, n,$$

where the index “env” refers to the environment. Entropy production in the circuit as a whole is

$$\Delta S_{\text{cir}} = \frac{1}{T} \sum_i h_i x_i. \quad (3.27)$$

The same amount of entropy is transferred to the environment and its accumulation there leads to the increase in entropy of an isolated system (the circuit plus the environment), given as

$$\Delta S_{\text{is}} = \frac{1}{T} \sum_i h_i x_i. \quad (3.28)$$

Hence, for the considered system the function value

$$\sum_i h_i x_i.$$

should be maximal. Then the following model becomes obvious:

Find

$$\max \sum_i h_i x_i \quad (3.29)$$

subject to

$$Ax = 0, \quad (3.30)$$

$$\sum_i H_i x_i - \sum_i h_i x_i = 0, \quad (3.31)$$

$$h_i = f_i(x_i), i = 1, \dots, n. \quad (3.32)$$

The right-hand side of the first Kirhchhoff law equation (3.30) is equal to zero due to the absence of sources and sinks ($Q = 0$) in the closed system. Equation (3.31) is the balance of produced and consumed energy in the circuit. The signs are chosen from the condition of thermodynamics that the removed heat ($\sum_i h_i x_i$) be negative.

If the closing relation is determined by expression (3.13), model (3.29)–(3.32) takes the following form:

Find

$$\max \sum_i z_i x_i^{\beta+1} \quad (3.33)$$

subject to

$$Ax = 0, \quad (3.34)$$

$$\sum_i H_i x_i - \sum_i z_i x_i^{\beta+1} = 0, \quad (3.35)$$

$$h_i = z_i x_i^\beta, \quad i = 1, \dots, n. \quad (3.36)$$

Comparison between (3.33) and (3.35) reveals the possibility of replacing the objective function (3.31) by the expression

$$\max \sum_i H_i x_i \quad (3.37)$$

and then formulating the following statement: The flows in a closed active hydraulic circuit are distributed so that the energy produced by sources of effective heads and, correspondingly, the energy consumed is maximal. This statement provides information about the physical regularities of flow distribution in circuits, in addition to information of the theorem concerning the least thermal action.

To analyze mathematical properties of model (3.33)–(3.36) we will write the Lagrange function of the circuit, representing preliminarily condition (3.34) in the form

$$\sum_{i \in I_j} a_{ij} x_i = 0, \quad j = 1, \dots, m-1, \quad (3.38)$$

where I_j is a subset of branches incident to node j .

Then the Lagrange function will be

$$L = \sum_{i=1}^n z_i x_i^{\beta+1} - \sum_{j=1}^{m-1} \lambda_j \sum_{i \in I_j} a_{ji} x_i + \lambda_m \left(\sum_{i=1}^n z_i x_i^{\beta+1} - \sum_{i=1}^n H_i x_i \right), \quad (3.39)$$

where λ_j and λ_m are Lagrange multipliers.

Let us take the derivative of (3.39) with respect to x_i and equate it to zero:

$$(\beta+1)(\lambda_m+1)z_i x_i^\beta + \lambda_{bi} - \lambda_{ei} - \lambda_m H_i = 0, \quad (3.40)$$

where λ_{bi} and λ_{ei} are multipliers for the initial and final nodes of branch I , respectively.

Since, at $H_i = 0$,

$$\lambda_{bi} - \lambda_{ei} = (\beta+1)(\lambda_m+1)z_i x_i^\beta = (\beta+1)(\lambda_m+1)h_i, \quad (3.41)$$

the difference of the Lagrange multipliers for nodes incident to the i th branch is proportional to the head loss in it.

The analytical expression for λ_m is obtained by addition of the derivatives $\partial L / \partial x_i$ for all i belonging to any closed loop k with effective heads. The sum will

have the form

$$(\beta + 1)(\lambda_m + 1) \sum_{i \in k} h_i - \lambda_m \sum_{i \in k} H_i = (\beta + 1)(\lambda_m + 1) \sum_{i \in k} H_i - \lambda_m \sum_{i \in k} H_i = 0. \tag{3.42}$$

(Equality to zero is explained by the equilibrium character of flow distribution). Expression (3.42) does not contain λ_j , since “ $+\lambda_j$ ” and “ $-\lambda_j$ ” vanish for each node j . From (3.42) it follows that

$$\lambda_m = -\frac{(\beta + 1)}{\beta}. \tag{3.43}$$

As $\beta > 0$, then $|\lambda_m| > 1$. For the linear closing relation ($\beta = 2$), $\lambda_m = -2$, and for the quadratic relation ($\beta = 2$), $\lambda_m = -1.5$. Since the multiplier λ_m is a derivative of the entropy with respect to the energy imbalance, its negativity is quite clear. If we could increase the energy of flows $\sum_i H_i x_i$ without an increase of its consumption $\sum_i z_i x_i^{\beta+1}$ and entropy production, then with respect to the equilibrium state

$$\sum_i H_i x_i = \sum_i z_i x_i^{\beta+1} \quad \text{and} \quad S = \max S$$

S of the system should have decreased.

Substituting (3.43) into (3.40) we will find that in a general case

$$\lambda_{bi} - \lambda_{ei} = \Delta\lambda_i = \lambda_m (H_i - h_i). \tag{3.44}$$

Depending on the choice of the $m - 1$ independent nodes the absolute values of λ_j ($j \neq m$) will vary, but the $\Delta\lambda_i$ will remain unchanged.

The second partial derivatives of L with respect to x_i are

$$\frac{\partial^2 L}{\partial x_i^2} = \beta(\beta + 1)(\lambda_m + 1) z_i x_i^{\beta-1} \leq 0,$$

since $\lambda_m < -1$. Hence, the solution to problem (3.33)–(3.36) corresponds to the maximum of $L = f(x)$ and the maximum of the objective function (3.33) for an admissible set of solutions. Fig. 3.3a illustrates the possibility of a maximum point to exist for the convex objective function. The objective function $a'b'$ that has the maximum F_{\max} is an intersection of the vertical surface drawn through a nonlinear admissible region of solutions to the problem (the region ab), perpendicular to the plane $x_1 x_2$, with the surface of the function $f(x)$ above this plane.

An *open active circuit* (with internal sources of effective heads and external sources and sinks) represents a thermodynamic system, whose conditions for interaction with the environment are determined by fixing enthalpy and pressure. In fact, the setting of the vector of nodal flows at fixed circuit resistance uniquely determines pressure (head) differentials between the points of sources and sinks, and between the energy flows as well. For both these and isolated systems, the maximum entropy is achieved at the equilibrium state. In this case the model of flow distribution takes the following form:

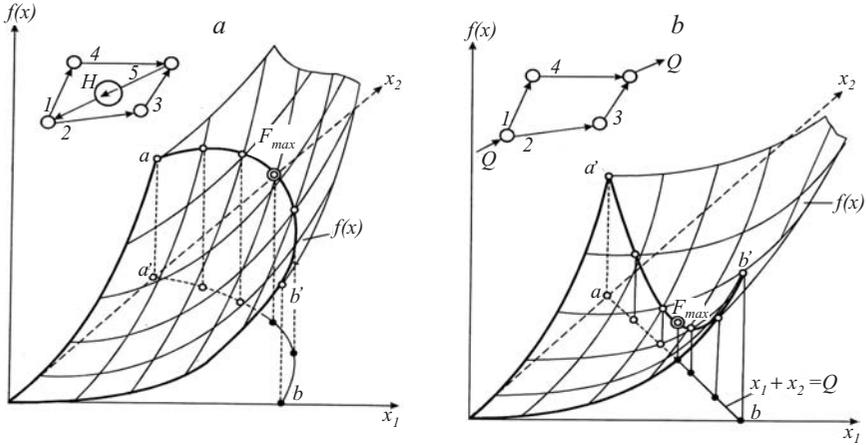


FIGURE 3.3. The objective function and the extremum points on the nonlinear (a) and linear (b) sets of constraints.

Find

$$\max \left(\sum_{j=1}^m P_j Q_j + \sum_{i=1}^n H_i x_i = \sum_{i=1}^n z_i x_i^{\beta+1} \right) \tag{3.45}$$

subject to

$$Ax = Q, \tag{3.46}$$

$$\sum_{j=1}^m P_j Q_j + \sum_{i=1}^n H_i x_i - \sum_{i=1}^n z_i x_i^{\beta+1} = 0, \tag{3.47}$$

$$P = e P_m - \bar{A}_g^{-1} (h_g - H_g), \tag{3.48}$$

Where P is a vector of heads at nodes $j = 1, \dots, m - 1$; P_m is the fixed head at node $j = m$; h_g and H_g are respective vectors of the head loss and the effective heads in branches of the “circuit tree” comprising the paths from nodes $j = 1, \dots, m - 1$ to node m ; \bar{A}_g^{-1} is a matrix of “paths” corresponding to this tree that is obtained by inversion of the submatrix of matrix A for branches of this tree; e is a unit vector.

The extreme thermodynamic model of a passive circuit can be obtained as a special case of models (3.33)–(3.36) and (3.45)–(3.48). This can be proved by mentally isolating a passive fragment with n_p branches and m_p nodes from the active circuit. The variables $x_i, i = n_p + 1, \dots, n$, on branches of the rejected circuit part include flows that determine directions and magnitudes of sources and sinks $Q_j, j = 1, \dots, m_p$, in the isolated fragment. Then conditions (3.47) and (3.48) are excluded and model (3.45)–(3.48) is replaced by model (3.10), constructed on the basis of the heat theorem. The Lagrange function in this case

has the form

$$L = \sum_{i=1}^{n_p} z_i x_i^{\beta+1} - \sum_{j=1}^{m-1} \lambda_j \left(\sum_{i \in I_j} a_{ji} x_i \right)$$

and its second derivatives are

$$\frac{\partial^2 L}{\partial x_i^2} = \beta(\beta + 1) z_i x_i^{\beta-1} \geq 0. \quad (3.49)$$

Hence, the extremum of $L(x)$ is the point of minimum, and thus the problem of entropy maximization is transformed to the problem of heat minimization, and the Kirchhoff–Maxwell theorem is deduced as a corollary of the second thermodynamics law with its extension to passive circuits. Coincidence of the form of objective functions in the “entropy” models (3.33)–(3.36) and (3.45)–(3.48) with the “energy” model (3.10) is due to the fact that the multiplier $1/T$ is removed from the maximized expression (3.10) on the assumption of constant temperature.

The revealed interrelation of flow distribution problems is a special case of the general thermodynamic law. It states that systems with constant energy tend to maximum entropy, and in systems in which fixation of any parameters results in energy exchange with the environment, the minimum of the corresponding energy kind is achieved. In the considered case of fixed flows of liquid (gas), which the circuit exchanges with its environment, we minimize mechanical energy consumption or, what is the same, quantity of heat liberated in the circuit.

Fig. 3.3a and b presents a graphical interpretation of the transformation of maximization problem to the minimization problem for the objective function that is convex on the unlimited set of variables.

Here we will not discuss thermodynamic interpretations of the models with regulated and distributed parameters that were considered in [81]. It should only be pointed out that such models can often be reduced to models with lumped parameters, as was explained above.

At the end of our discussion of homogeneous circuits let us show that the extremality criterion (3.11) that was justified above using the principle of virtual works, can be obtained from thermodynamic model (3.33)–(3.36). To do this we perform elementary transformations of the partial Lagrange function:

$$\begin{aligned} L &= \sum_{i=1}^n z_i x_i^{\beta+1} + \lambda_m \left(\sum_{i=1}^n z_i x_i^{\beta+1} - \sum_{i=1}^n H_i x_i \right) \\ &= - \sum_i \frac{\beta + 1}{\beta} \left(\frac{z_i x_i^{\beta+1}}{\beta + 1} - H_i x_i \right) = \text{const} \sum_i \left(\frac{f_i(x_i) x_i}{\beta + 1} - H_i x_i \right). \end{aligned}$$

Of course, the constant may be removed from the extremality criterion.

The analysis presented in this section and the previous portion of the book show that extreme models of homogeneous circuits can be constructed on the basis of two competitors: a) the second law of thermodynamics and the principle of virtual works to describe stationary (or nonstationary, if the time variable is excluded from

the analysis) flows; and b) the second law and the principle of the least action to describe liquid flow using the time coordinates.

The thermodynamic analysis of closing relations is given in the next section. This section will conclude with several examples of applying thermodynamic models.

Examples of Calculations

Agreement between the solutions of the problem (3.33)–(3.36) and the system of the Kirchhoff equations (3.6)–(3.8) is tested on a number of examples. Table 3.2 presents the calculation results for the circuit presented in Fig. 3.4.

Consideration was given to three variants:

1. the quadratic closing relation $h_i = z_i x_i^2$ for all $i = 1, \dots, n$;
2. the linear closing relation $h_i = z_i x_i$ for all $i = 1, \dots, n$;
3. the quadratic closing relation $h_i = z_i x_i^2$ for all $i = 1, \dots, 15$; $h_{16} = z_{16} x_{16}$.

The effective heads for the three variants are assumed to be equal: $H_5 = 90$; $H_{10} = 60$; $H_{12} = 100$. The resistances z_i of branches coincide for variants 1. and 3. and in variant 2. they are chosen to be 1000 times lower.

For the given circuit the extreme problem solution proved to satisfy the Kirchhoff laws in all the considered variants. It is also valid in case the laminar and turbulent modes of motion are simultaneously present in the circuit (variant 3.).

3.4. Thermodynamic Interpretations of Hydraulic Circuit Theory: Heterogeneous Circuits

Problem Urgency

The theoretical and practical significance of flow distribution calculation in circuits with multiphase chemically reacting flows is conditioned, for example, by the following problems:

- analysis of conditions for self-ignition of combustible components in systems of harmful industrial waste disposal;
- calculation of depositions of heavy hydrocarbons in systems for transporting oil, oil products, and natural gas;
- determination of conditions for condensate formation in long-distance steam pipelines;
- assessment of concentrations of harmful substances in ventilation and air conditioning systems in residential dwellings and in public and industrial places;
- hydraulic calculations of chemical reactors;
- calculation of the schemes of energy carrier travel at energy plants with compound flows (at electrochemical energy converters, integrated gasification combined-cycle power plants, etc.).

Further successful development of the heterogeneous circuit theory will certainly offer many new spheres of its application.

TABLE 3.2. Calculations Results of the Circuit

Branch	z_i	x_i	h_i	$\Delta\lambda_i$	Independent node	λ_j
<i>Variant 1</i>						
1	$0.78 \cdot 10^{-4}$	799	49.8	—	1	74.7
2	$0.25 \cdot 10^{-3}$	199	9.9	14.9		
3	$0.64 \cdot 10^{-4}$	397	10.1	15.1	2	89.6
4	$0.12 \cdot 10^{-3}$	404	19.6	29.4		
5	$0.64 \cdot 10^{-4}$	397	10.1	119.8	3	104.7
6	$0.70 \cdot 10^{-2}$	100	70.0	104.7		
7	$0.24 \cdot 10^{-3}$	501	60.2	90.5	4	75.3
8	$0.28 \cdot 10^{-4}$	597	10.0	15.0		
9	$0.64 \cdot 10^{-4}$	400	10.2	—	5	-44.5
10	$0.64 \cdot 10^{-4}$	399	10.2	—		
11	$0.18 \cdot 10^{-2}$	197	69.9	104.9	6	60.2
12	$0.10 \cdot 10^{-4}$	1001	10.0	135		
13	$0.28 \cdot 10^{-4}$	601	10.1	15.1	7	-30.3
14	$0.20 \cdot 10^{-2}$	200	80	119.8		
15	$0.50 \cdot 10^{-3}$	200	20	30	8	-15.3
16	$0.10 \cdot 10^{-2}$	97	9.4	14.2	$\lambda_m = -1.5$	
<i>Variant 2</i>						
1	$0.78 \cdot 10^{-1}$	506	39.5	—	1	79.0
2	0.25	111	27.7	55.3		
3	$0.65 \cdot 10^{-1}$	155	9.9	19.8	2	134.3
4	0.12	233	27.9	55.8		
5	$0.64 \cdot 10^{-1}$	72	4.6	170.8	3	154.1
6	$0.70 \cdot 10$	11	77.0	156.1		
7	0.24	251	60.1	120.2	4	98.3
8	$0.28 \cdot 10^{-1}$	230	6.4	12.8		
9	$0.64 \cdot 10^{-1}$	186	11.9	—	5	-72.5
10	$0.64 \cdot 10^{-1}$	320	20.5	—		
11	$0.18 \cdot 10$	44	79.2	158.1	6	83.6
12	$0.10 \cdot 10^{-1}$	462	4.62	190.7		
13	$0.28 \cdot 10^{-1}$	262	7.3	14.7	7	-36.6
14	$0.20 \cdot 10$	43	86.0	170.8		
15	0.50	75	37.5	75.1	8	-23.8
16	$0.10 \cdot 10$	18	18	35.9	$\lambda_m = -2.0$	
<i>Variant 3</i>						
1	$0.78 \cdot 10^{-4}$	800	49.9	—	1	74.9
2	$0.25 \cdot 10^{-3}$	202	10.2	15.3		
3	$0.64 \cdot 10^{-4}$	400	10.2	15.3	2	90.2
4	$0.12 \cdot 10^{-3}$	351	14.8	22.1		
5	$0.64 \cdot 10^{-4}$	463	13.7	114.4	3	105.5
6	$0.70 \cdot 10^{-2}$	97	65.9	98.3		
7	$0.24 \cdot 10^{-3}$	522	65.4	98.2	4	83.4
8	$0.28 \cdot 10^{-4}$	602	10.1	15.2		
9	$0.64 \cdot 10^{-4}$	404	10.4	—	5	-31.0
10	$0.64 \cdot 10^{-4}$	396	10.0	—	—	—
11	$0.18 \cdot 10^{-2}$	198	70.6	105.9	6	67.3
12	$0.10 \cdot 10^{-4}$	953	9.1	136.4		
13	$0.28 \cdot 10^{-4}$	619	10.7	16.1	7	-30.9
14	$0.20 \cdot 10^{-2}$	195	76.1	114.4		
15	$0.50 \cdot 10^{-3}$	202	20.4	30.6	8	-15.7
16	$0.10 \cdot 10^{-2}$	171	0.17	0.1	$\lambda_m = -1.5$	

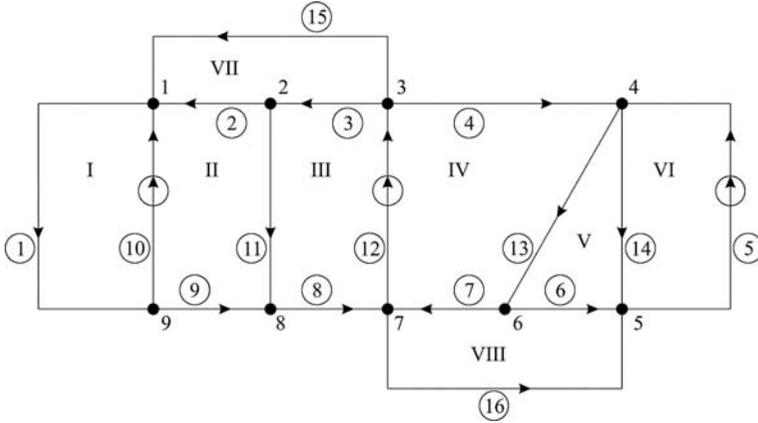


FIGURE 3.4. The calculated circuit scheme. Figures in circles are numbers of branches; 1–9 are numbers of nodes; I–VIII are numbers of loops; arrows in circles are effective heads; arrow show given direction of flow.

In terms of development of extreme thermodynamics models it is precisely the heterogeneous circuits that are the most interesting part of HCT, since presence of chemical reactions makes the problems of searching for the regions of thermodynamic attainability and partial equilibria highly topical¹.

Mathematical Model of a Heterogeneous Network

A model of the closed active heterogeneous network can be represented in a form similar to model (3.33)–(3.36) of the homogeneous system:

Find

$$\max \sum_{i=1}^n \frac{z_i x_i^{\beta+1}}{T_i} \tag{3.50}$$

subject to

$$Ax = 0, \tag{3.51}$$

$$\sum_{i=1}^n H_i x_i - \sum_{i=1}^n h_i x_i = 0, \tag{3.52}$$

$$h_i = z_i x_i^\beta, \quad i = 1, \dots, n, \tag{3.53}$$

$$x_i = (x_{i1}, \dots, x_{ik})^T, \tag{3.54}$$

$$z_i = f_i(\rho_i(x_i, T)), \tag{3.55}$$

$$H_i = \phi_i(\rho_i(x_i, T)). \tag{3.56}$$

¹ Note: There are many publications on the kind of two-phase flows that do not experience phase transitions and chemical transformations (transport of crushed solid material in water or air, transport of coal in methanol, etc). We do not deal with such flows.

The functional dependences (3.53) and (3.56) indicate that the heterogeneous circuits belong to the models with distributed parameters. In order to reveal properties of system (3.50)–(3.56) and possibilities of its reduction (approximation) to the model with lumped parameters, first, one must study the character of the closing relations (3.53). Such a study is the major subject of this section.

Thermodynamic Analysis of Closing Relations

Availability of physically and mathematically valid closing relations makes it possible to conduct a qualitative physical and mathematical analysis of diverse heterogeneous circuits. For example, these closing relations enable one to determine conditions for occurrence of multiphase flows, possible changes in the type of *piezometric plots* (graphical relationships between head loss and branch length) at chemical transformations and phase transitions, reasons for the many-valued solutions to a flow distribution problem, and so on.

When we derived the closing relations for multicomponent and multiphase flows, we took as the basis premise the equilibrium between different phases, which, in turn, is determined by the equality of chemical and other potentials.

Originally the idea of thermodynamic analysis of relationships between head losses and flow was tested on the example of a homogeneous isothermal flow of incompressible liquid. We considered the phase equilibrium between two conditional flows: a turbulent tube and an annular laminar layer surrounding it: The two move uniformly and in the same direction relative to one another. Thus, the *true* picture of vortex formation and increase in the flow turbulence degree with the growth of flow velocity was substituted by an *imaginary* picture of continuous growth of the turbulent tube diameter d_t from zero to d . The authors borrowed the idea of conditional flows from Landau's theory of quantum liquids [120], in which Landau used the concept of *conditional superfluid* and *normal flow*.

Since the studied flows are homogeneous and isothermal, we naturally reduced the equality of chemical potentials to the equality of hydraulic potentials, namely pressures, and correspondingly, to the equality of pressure losses in the turbulent tube (ΔP_t) and the laminar flow (ΔP_l) between any two tube cross-sections. The value of ΔP_t was calculated by the Darcy–Weisbach formula (1.55) and the Schifrinson formula was applied to determine the friction coefficient

$$\lambda_t = 0.11 (k/d_t)^{0.25}, \quad (3.57)$$

where k is a roughness coefficient.

When ΔP_l was determined by (1.55), the equivalent diameter d_l of the laminar ring and the coefficient λ_l were calculated from the expressions [3]:

$$d_l = 4 \frac{\bar{\omega}}{h} = 4 \frac{\pi (d^2 - d_t^2)}{4\pi (d + d_t)} = d - d_t, \quad (3.58)$$

$$\lambda_l = \frac{A}{Re} = \frac{96\nu}{w(d - d_t)}, \quad (3.59)$$

where $\bar{\omega}$ and h are the cross-sectional area of the ring and its perimeter, respectively; A is a form coefficient; Re is a Reynolds number; ν is the kinematic viscosity.

From transforming the equality

$$\Delta P_t = \Delta P_l$$

by means of formulas (1.55) and (3.57)–(3.59), we determined the following relationships:

$$\Delta P = z x^2 = \frac{0.108 k^{0.25} l}{f(d_t(w)) \rho} x^2, \tag{3.60}$$

$$f(d_t) = d_t^{1.25} (0.6 d_t^2 + 0.5 d^2)^2. \tag{3.61}$$

Comparison of the results calculated by equations (3.60) and (3.61) for pressure losses with water flow in tubes with different diameters to the reference data revealed the close agreement of the two sets of data, which confirmed to some extent the effectiveness of thermodynamic analysis of closing relations.

Multicomponent flows will be addressed now. We start with chemically homogeneous moving media subject to phase transitions. The difference in chemical potential is the driving force for both phase transitions and chemical transformations. Physical and mathematical descriptions of both processes should be similar.

Motion of a condensing ideal gas is the simplest example. As distinct from the analysis of incompressible liquids and homogeneous gases, the assumption of an isothermal flow is inadmissible here. First, if only the gas phase is present in the flow at the initial instant of motion, its conversion to liquid as a result of the isothermal process is impossible (see the isotherm 1–1 in Fig. 3.5). Second, in regions of phase transition, isotherms coincide with isobars, i.e., pressure also remains constant simultaneously with temperature (the isotherm 2–2 in Fig. 3.5), and therefore the process of medium motion becomes impossible.

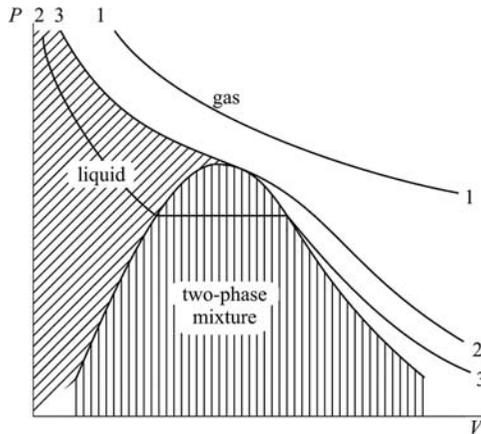


FIGURE 3.5. The diagram of substance state in the coordinates P, V .

Therefore, the flow was assumed to be *polytropic*. For ideal gases the *polytropic equation* has the form

$$PV^\gamma = \text{const.} \quad (3.62)$$

For the adiabatic process we have

$$\gamma = \frac{c_p}{c_v}, \quad (3.63)$$

where c_p and c_v are the isobaric and isochoric heat capacities, respectively. When γ tends to unity, the process is isothermal at its limit.

The next supposition was that the moving medium represents a spatially homogeneous mixture of gas and suspended fog droplets.

Density of such a medium is determined from the expression

$$\rho = \frac{x}{(x - x_c)\rho_g^{-1} + x_c\rho_c^{-1}}, \quad (3.64)$$

where x is the mass flow; and the indices c and g refer to condensed and gas phases, respectively.

Since at moderately high flow pressures

$$\rho_g \ll \rho_c,$$

equation (3.64) can be replaced by the approximate expression

$$\rho = \frac{\rho_g x}{(x - x_c)}. \quad (3.65)$$

The closing relation for the polytropic flow of condensing ideal gas (the flow of the condensed phase at the initial cross-section of tube is equal to zero) can be determined from the Darcy–Weisbach equation written in the differential form

$$-dP = \frac{\lambda \rho w^2}{2d} dl. \quad (3.66)$$

To substitute the variable w by the mass flow x we will express the density ρ at an arbitrary flow cross-section via the density ρ_1 at the initial state.

From the polytropic equation (3.62) follows

$$\rho_g = \rho_{g1} \left(\frac{P}{P_1} \right)^{1/\gamma}, \quad (3.67)$$

since $\rho = 1/v$.

In terms of (3.65) we have

$$\rho = \rho_1 \left(\frac{P}{P_1} \right)^{1/\gamma} \frac{x}{(x - x_c)}. \quad (3.68)$$

Since

$$x = 0.25w\rho\pi d^2,$$

then

$$-dP = \frac{8\lambda P_1^{1/\gamma} x(x - x_c)}{\pi^2 \rho_1 d^5 P^{1/\gamma}} dl. \quad (3.69)$$

Let us introduce the notation

$$\psi = \frac{8\lambda P_1^{1/\gamma}}{\pi^2 d^5 \rho_1}. \quad (3.70)$$

Then

$$\int_{P_2}^{P_1} P^{1/\gamma} dP = \int_0^l \psi x(x - x_c) dl$$

and

$$P_1^{(\gamma+1)/\gamma} - P_2^{(\gamma+1)/\gamma} = \varphi x(x - x_c)l, \quad (3.71)$$

where

$$\varphi = \psi \frac{(\gamma + 1)}{\gamma}. \quad (3.72)$$

Expression (3.71) is an integral form of the closing relation for the “ideal” two-phase flow from which the final pressure is determined:

$$P_2 = \left(P_1^{(\gamma+1)/\gamma} - \varphi x(x - x_c)l \right)^{\gamma / (\gamma+1)}. \quad (3.73)$$

The closing relation for the single-phase flow ($x_c = 0$) is derived as a particular case of (3.71), namely,

$$P_1^{(\gamma+1)/\gamma} - P_2^{(\gamma+1)/\gamma} = \varphi x^2 l, \quad (3.74)$$

and at $\gamma = 1$ it transfers to the known formula for the isothermal gas flow,

$$P_1^2 - P_2^2 = \varphi x^2 l. \quad (3.75)$$

At the same time equation (3.71) is not symmetric relative to phase transitions: gas \rightarrow liquid; and liquid \rightarrow gas. When the gas phase flow rate ($x = x_c$) is equal to zero, the pressure loss in the branch also turns to zero, which is certainly incorrect theoretically. This property of the determined closing relation is quite clear, as it was derived by the ideal gas state equation. But in principle this equation is not adequate for the description of condensed phases. However, when the gas phase disappears in the flow the errors in determination of pressure losses by equation (3.71) are practically negligible. This is due to the fact that the condensate density at a distance from the critical point is much higher than the gas density, and the value of ΔP sharply decreases with condensation. If the tube diameter were chosen with the proviso that a single-phase gas flow passed through it, then, with motion of the same condensate mass in it, ΔP would approach zero.

Let us mention an easily comprehensible fact, namely, that the phase transitions (and the chemical transformations) can lead to both convex (Fig. 3.6, curve 3)

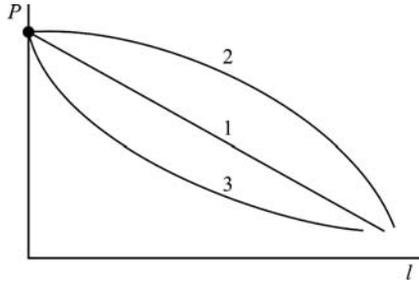


FIGURE 3.6. Possible forms of piezometric plots

and concave (curve 2) forms of the piezometric plots $P = f(l)$. The convex form takes place when the increase of substance density due to condensation exceeds the decrease of ρ as a result of gas expansion.

It is clear that the application of equation (3.71) to practical calculations requires an iterative adjustment of P_2 by determining x_c from the phase equilibrium conditions.

In principle, the closing relation for the polytropic flow of real gas that is obtained by the van der Waals equation (or some other state equation) may be taken with some or another degree of error for calculation of individual components of the vector x_i .

The polytrope equation of the van der Waals gas has the form

$$(P + a\rho^2)(1/\rho - b)^{\gamma} = \text{const.} \tag{3.76}$$

Since, analytically, it is difficult to integrate the Darcy–Weisbach formula

$$-dP = \frac{0.811\lambda x^2}{d^5\rho} dl \tag{3.77}$$

($0.811 \approx 8/\pi^2$; see, for example, equation (3.69)) with respect to ρ , let us preliminarily decompose the pressure by powers of density:

$$P(\rho) = P(\rho_1) + P'(\rho_1)(\rho - \rho_1) + 0.5P''(\rho_1)(\rho - \rho_1)^2 + 0.167P'''(\rho_1)(\rho - \rho_1)^3. \tag{3.78}$$

Preliminary calculations have shown that the four terms of decomposition (the coefficient of the fourth term is assumed to have a rounded-off value) are sufficient to determine two roots of equation (3.77), obtained as a result of integration to have real values in the region of phase transitions. The determined closing relation has the form

$$a_1(\rho_1^4 - \rho_2^4) + a_2(\rho_1^3 - \rho_2^3) + a_3(\rho_1^2 - \rho_2^2) = \varphi x^2 l, \tag{3.79}$$

where

$$a_1 = 0.125P'''(\rho_1),$$

$$a_2 = 0.333(P''(\rho_1) - 1.022P'''(\rho_1)\rho_1)$$

and

$$a_3 = 0.5 (P'(\rho_1) - P''(\rho_1)\rho_1 + 0.501P'''(\rho_1)\rho_1^2).$$

It is obvious that for the single-phase flow of ideal gas the second and third derivatives of pressure with respect to density turn out to be zero and equation (3.79) converts to the quadratic relation (3.75).

It is of no doubt that the terms of no lower than the third power should be present in the algebraically expressed closing relations for any flows experiencing phase transitions. Indeed, the region of phase transitions in the state diagrams lies below the critical point, at which the first and second derivatives of pressure with respect to the volume (density) equal zero. This point can be determined only by the equations in which two first derivatives do not vanish identically.

Analytical dependences between pressure loss and flow for chemically reacting flows can be determined only at the limiting idealization of the studied process. To have a clear picture of chemical transformation influence on liquid flow we should also exclude from mathematical description of the problem all factors that are not directly related to transformations of substances (e.g., changes in medium density with variation in temperature and pressure).

Based on the indicated requirements we will consider an isothermal flow of two liquid incompressible isomers 1 and 2 as a model example. In the flow the first component is converted to the second as a result of a *monomolecular reaction of the first order*, i.e., a reaction corresponding to the equation,

$$\frac{dx_1}{d\tau} = -kx_1, \quad (3.80)$$

where x_1 is a mole fraction of component 1, and k is a rate constant of the reaction.

In this case the flow density ρ is determined by the equation

$$\rho = \left(\left(\frac{1}{\rho_2} - \frac{1}{\rho_1} \right) x_2 + \frac{1}{\rho_1} \right)^{-1}, \quad (3.81)$$

x_2 is calculated from the material balance equation

$$x_1 + x_2 = 1, \quad (3.81a)$$

and the solution to equation (3.80) is

$$x_1 = e^{-k\tau}, \quad (3.82)$$

which is true provided that for $\tau = 0$, $x_1 = 1$ and $x_2 = 0$,

$$x_2 = 1 - e^{-k\tau}. \quad (3.83)$$

In terms of (3.83), equation (3.81) can be transformed as

$$\rho = \left(\frac{1}{\rho_2} + \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right) e^{-k\tau} \right)^{-1}. \quad (3.84)$$

If the form of the function $\rho = f(\tau)$ is known, the relationships between ΔP and x can be found from the Darcy–Weisbach equation

$$-dP = \frac{\lambda w^2(\rho) \rho(\tau)}{2d} dl(\rho(\tau)) = \frac{8\lambda x^2}{\pi^2 d^5 \rho(\tau)} dl(\rho(\tau)). \quad (3.85)$$

Integration of (3.85) results in

$$\Delta P = \frac{32\lambda x^3}{\pi^3 d^7} \left[\frac{\tau}{\rho_2^2} + \frac{2}{k\rho_2} \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right) (1 - e^{-k\tau}) + \frac{1}{2k} \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right)^2 (1 - e^{-2k\tau}) \right]. \quad (3.86)$$

Expression (3.86) represents the dependence of pressure loss on the time of liquid motion between the pipeline section that is taken as initial and the current section. However, before passing to the thermodynamic analysis the variable τ should be excluded, i.e., it is necessary to find a relation between ΔP and x at the fixed l that is revealed for the flows with phase transitions. To solve this problem, first the form of the function $l = f(\tau)$ is determined:

$$dl = w(\rho(\tau)) d\tau, \\ l = \frac{4x}{\pi d^2} \left[\frac{\tau}{\rho_2^2} + \frac{1}{k} \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right) (1 - e^{-k\tau}) \right]. \quad (3.87)$$

Then a simple transformation of equation (3.86) is performed:

$$\Delta P = \frac{32\lambda x^3}{\pi^3 d^7} \left[\frac{\tau}{\rho_2^2} + \frac{1}{k\rho_2} \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right) (1 - e^{-k\tau}) \right] \\ + \frac{32\lambda x^3}{\pi^3 d^7} \left[\frac{1}{k\rho_2} \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right) (1 - e^{-k\tau}) + \frac{1}{2k} \right. \\ \left. \times \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right)^2 (1 - e^{-2k\tau}) \right]. \quad (3.88)$$

Comparison of (3.87) and (3.88) clearly shows that pressure loss ΔP can be represented as the sum of the term depending on l and the one independent of l :

$$\Delta P = \frac{\varphi x^2 l(\tau)}{\rho_2} + [\psi_1 (1 - e^{-k\tau}) + \psi_2 (1 - e^{-2k\tau})] x^3. \quad (3.89)$$

The first term on the right-hand side of (3.89) coincides with classical expressions of closing relations for circuits with lumped parameters, provided the pipe length and the time for the liquid to pass through it are fixed and the liquid density equals the density of the second isomer (the final reaction product). The second term is a correction for the value of ΔP that is determined by the change in density of the moving medium because of the chemical reaction.

Equation (3.89) shows that when τ and l are equal to zero, ΔP also vanishes. At $\tau \rightarrow \infty$ the relationship $\Delta P = f(l)$ tends to become linear. This conclusion is

clear, since the chemical transformations are completed in an infinitely long time period and the density becomes constant. The sign of “chemical” correction for the variation in ΔP depends on the sign of difference $1/\rho_1 - 1/\rho_2$, i.e., on the density variation during reaction. If the density of the final product ρ_2 exceeds ρ_1 , then $\Delta P = f(l)$ on the initial branch section is concave. At $\rho_2 < \rho_1$ the function $\Delta P(l)$ becomes convex. The function $P(l) = P^1 - \Delta P(l)$ is naturally convex when $\rho_2 > \rho_1$ and concave at $\rho_2 < \rho_1$ (see Fig. 3.6).

Note that both the “chemical” and “phase” corrections are cubic (or higher-power) functions of the flow. This fact can be explained physically, since the impact of chemical transformations on hydrodynamics is similar to the impact of phase transitions and is determined solely by the change in the flowing medium density (if the possible variation in viscosity is neglected). Therefore, the mathematical descriptions of the effects of these processes on liquid (gas) flow should also be similar. The impossibility of applying closing relations of a power lower than the third power for flows with a variable phase composition was shown above. The same is naturally true of chemically reacting liquids.

Based on what is said above, let us represent the closing relation (3.89) in a “more thermodynamic” form, excluding from it the time variable that is uniquely related with ρ_1 , ρ_2 and l at the fixed x :

$$\Delta P = \varphi_1(\rho_2, l)x^2 + \varphi_2(\rho_1, \rho_2)x^3. \quad (3.90)$$

For the strict derivation of expressions (3.89) and (3.90) we introduced very severe constraints into the initial problem statement. It is clear, however, that the area of qualitative analysis using the obtained equations can be considerably extended in comparison with the area formally corresponding to the accepted mathematical model. Thus, the initial and final compositions of flows can be assumed to be not pure substances, but mixtures and equation (3.81a) in a general form can be supposed to describe a linear material balance. For the flows with $\rho = f(P, T)$ it is natural to assume that the right-hand side of equation (3.90) represents only the two first terms of a more complicated relation that probably includes terms of a powers higher than the third with respect to x .

The obtained closing relations can be applied to show that at least at $k \ll 1$, the property of “cost function slight slope along the head axes” that was established by V.Ya. Khasilev, does not change essentially at a transition from the flows of incompressible media to the chemically reacting flows (see Section 3.3). Indeed, with the indicated constraint on the reaction rate constant, time τ during which the liquid passes the distance l is expressed approximately by

$$\tau \approx \text{const} \frac{d^2}{x},$$

and the dependence $\Delta P = f(x)$ becomes close to quadratic, which was assumed by V.Ya. Khasilev. It may be supposed that at certain constraints the properties of

cost functions of pipeline networks that were determined in [76, 106] hold for the multiphase flows as well.

A fundamental character of closing relations (availability of a “lumped” component of the second power and corrections of higher powers) will apparently not change at a transition from complete to partial equilibria in flows. However, a complex analytical type of these relations indicates that in practical calculations of heterogeneous circuits they should be either determined by the iterative computational procedures or indirectly accounted for at approximation of the models of hydraulic systems on the whole (see below).

In concluding the analysis of closing relations, we will briefly address their derivation for nonsteady flow distribution. The analysis can be based on equation (3.25). The terms of its right-hand side are naturally interpreted as the stationary (the first term) and the nonstationary (the second term) components of head losses.

It is obvious that when we study a steady process, the second term turns out to be equal to zero and equation (3.25) reduces to the traditional form of the closing relation (3.13). Certainly, if the change in the “steady form” for the flows with phase transitions and chemical transformations is taken into account, it seems natural to replace (3.25) by the more general expression

$$h_i(\tau) = f_i(x_i, \tau) + \psi_i \frac{dx_i(\tau)}{d\tau}, \quad (3.91)$$

where the form of terms on the right-hand side is determined by the properties of the moving medium (gas, heterogeneous mixture of gas and condensed particles) and the character of processes running in the flows (phase transitions, chemical reactions, friction, heat exchange, etc.).

The problem of determining the expression for the first term was tackled to a considerable extent above. The problem of searching for the second term form will be not discussed in this book. It should be a subject of independent extensive studies. It should be noted, only, that depending on the disturbance nature the derivative $dx_i(\tau)/d\tau$ in (3.91) may be substituted by the derivative of pressure or temperature, the sum of derivatives of individual components of the vector flow in branch i , and so on.

On the whole the thermodynamic analysis of nonsteady flow distribution proves to be useful, when we are interested in the *results* of transient processes rather than in the *time* of their occurrence, which was considered above. For example, in the analysis of impact of the fast operation of stop valves in a pipeline network, it is important to determine a maximum liquid pressure and to check whether it exceeds an admissible value or not. The question the matter of what fraction of a second or of what seconds such pressure arises—is not so important (if, of course, the choice of the maximum rate of stop valve operation is not dealt with). In the studies of processes of heavy hydrocarbons, precipitation in gas and oil pipelines, or soot in tubes of chemical reactors, thermodynamics helps determine maximum precipitation of harmful substances relative to hourly mass flow of the moving medium and then estimate tentatively the time of tube “overgrowing.” At least in a number of cases it is more important to determine the probability that explosive mixtures

are formed in communications of energy or other industrial plants than to find the time taken for the corresponding reactions to proceed under favorable conditions.

Examples of Heterogeneous Circuit Application

The methods of constructing thermodynamic models of heterogeneous hydraulic systems to solve applied problems will be illustrated by two examples: 1) *fire spread* in complex air exchange systems; and 2) burning and disposal of harmful pollutants of industrial plants.

Prior to direct modeling of fire spread we will briefly address the topical problem of analysis of normal operation conditions for air exchange systems. This subject was touched upon in [91].

Ventilation and air conditioning systems for residential and industrial premises should provide both the requisite sanitary standards in temperature and moisture and the acceptable chemical composition of air. Whereas until recently the main method of controlling harmful emissions on premises was the intensive dilution of indoor air with outdoor air, now such a purification method may be dangerous. This is because in the “purifying” outdoor air the concentrations of harmful substances may be much higher than the (admissible) standards. Since indoor and outdoor temperature and moisture usually differ considerably, chemical composition of air flows in any building changes significantly. These changes can be calculated by modeling the air exchange systems on the basis of heterogeneous hydraulic circuits.

Modeling of fires in air exchange systems is the most sophisticated and theoretically interesting case when we attempt a “chemical and hydraulic” description of the system. Such systems include ventilation networks of buildings and other structures (such as mines and subways). The appropriate models, if available, will supposedly contribute to working out preventive measures and improving fire control.

The mathematical modeling of fires has been the subject of numerous publications (see, for example, [66]). Originality of the authors’ approach consists in the network problem statement and its presentation in terms of HCT and thermodynamics.

Prior to solution of such a complex problem currently we can create just a draft model that should be adjusted successively in the course of further studies.

To make the presentation clear we will first describe fires on the basis of a loop system of hydraulic circuit equations that is similar to system (3.6)–(3.8) and apply it in combination with MEIS; then we will show how to pass from this system to nodal potentials and the extreme model (3.50)–(3.56).

We will not construct equivalent calculated schemes of a real object, and we will suppose that the air exchange scheme (hydraulic circuit) is known. A simplest open double-loop hydraulic circuit is chosen as an example (Fig. 3.7a). Assume that the fire occurs on branch 2 and can spread to the rest of the scheme. The difference in densities on individual circuit branches induces gravitational heads denoted by H_{g1} and H_{g2} .

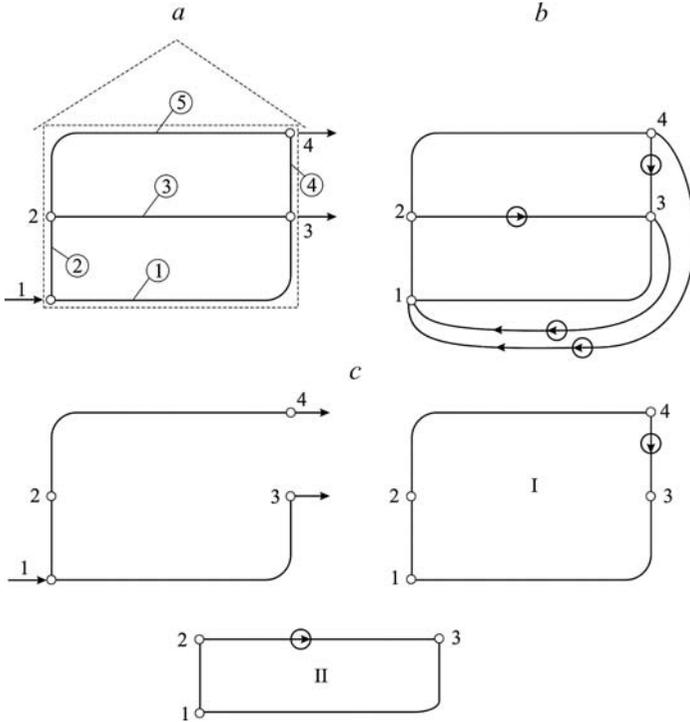


FIGURE 3.7. Hydraulic circuit schemes. *a*) basic calculated scheme, *b*) scheme to study relationships between Q and H_g ; *c*) spanning tree and calculated circuit loops. Figures in circles are numbers of branches.

It is clear that if the sources and sinks at nodes of the calculated scheme are not regulated, they are to change with the change in H_g . We can study relationships between the vectors of sources (sinks) Q and the gravitational heads H_g substituting the scheme in Fig. 3.7*a* by the scheme in Fig. 3.7*b*. Here the effective heads of branches 3–1 and 4–1 are taken equal to the pressure difference between the windward and leeward sides of the modeled object. However, the latter scheme will not be used in the theoretical analysis, though in practical calculations similar transformations of schemes may turn out to be necessary. We select loops I and II as independent (Fig. 3.7*c*), which correspond to chords 4 and 3, which were determined as a result of constructing of the spanning tree presented in Fig. 3.7*c*.

The loop system of equations for the considered hydraulic circuit can be represented as:

$$Ax = Q, \tag{3.92}$$

$$Bh = BH_g, \tag{3.93}$$

$$h_i = f_i(x_i, \rho_i(x_i, T_i)), i = 1, \dots, 5, \tag{3.94}$$

$$H_{gk} = f_k(z_k, \Delta\rho_k), k = 1, 2, \quad (3.95)$$

$$T_i = T_i(\Delta T), \Delta T_i = T_{bi} - T_{ei} = \varphi_i(\alpha_i, F_i, T_{\text{env}}), \quad (3.96)$$

$$x_i = (x_{i1}, \dots, x_{ie})^T = \psi_i(y, T_i, P_i), \quad (3.97)$$

where H_g is a vector of the gravitational heads; z_k and $\Delta\rho_k$ are, respectively, the difference of geodetic level marks and the difference of densities of the upward and downward flows in the k th loop; T_{bi} and T_{ei} are temperatures at the inlet and the outlet of the i th branch; T_{env} is an environmental temperature; α_i and F_i are the heat transfer coefficient and the heat exchange surface on the i th branch.

A natural idea of computational algorithms is to construct a circuit model with lumped parameters (3.6)–(3.8) for iterative calculations instead of model (3.92)–(3.97) to adjust the values of components in the vectors x_i and H_g at each iteration.

It seems reasonable to calculate “normal” (before the fire) flow distribution at the first iteration, then to calculate fire on branch 2 and adjust chemical composition, gravitational heads, averaged temperatures, and densities of the moving medium. There are several variants for choosing the model for determination of combustion results, e.g.: 1) stoichiometric description of a small number of basic reactions; 2) determination on MEIS of the final equilibrium point x^{eq} at the given vector y , the given list of the components x and the fixed enthalpy H and pressure P ; 3) MEIS application to search for x^{ext} with the same data, as in the second variant, and the setting of the objective function that is the sum of concentrations of the most dangerous substances.

The first stoichiometric variant is the least suitable for assessing fire impact. However, successive sophistication of the considered model and determination of relationships between the mathematical properties and the assumptions made will make it possible to apply the stoichiometric model. Expediency of using the third model (the main block of MEIS – x^{ext}) is due at least to the fact that we are interested in both the fire spread over the circuit branches and the spread of harmful substances beyond its direct zone that can cause poisoning of people at certain concentrations.

Gravitational heads at the first approximation can be determined by the simplest relation

$$H_{gk} = z_k(\rho_{ck} - \rho_{hk}), \quad (3.98)$$

where ρ_{ck} and ρ_{hk} are the average densities of the upward and downward flows in the k th loop, respectively. They are given by

$$\rho_{ck} = \frac{1}{z_k} \sum_{i \in I_{ck}} \rho_i z_i, \rho_{hk} = \frac{1}{z_k} \sum_{i \in I_{hk}} \rho_i z_i, \quad (3.99)$$

where ρ_i and z_i are the average density and the difference of marks along the vertical axis for the i th branch, respectively; I_{ck} and I_{hk} are sets of branches with the downward (ck) and upward (hk) flows.

Temperatures of the branches and their variations can also be determined the linear approximation from the equations:

$$q_i = \alpha_i F_i (T_i - T_{\text{env}}) \tau, \quad T_i = 0.5 (T_{bi} + T_{ei}), \quad (3.100)$$

$$q_i = c_i x_i (T_{bi} - T_{ei}) \tau, \quad (3.101)$$

where q_i are heat losses to the environment on the i th branch, and c_i is the specific heat of the multicomponent flow. The estimated time τ corresponding to the supposedly dangerous rate of fire spread should be varied, apparently, to analyze real objects. In terms of the construction principles of thermodynamic models, τ does not belong to the variables sought in the problem.

In addition, the heat balance equations for the circuit as a whole should be satisfied:

$$\bar{A}_b C_b T_b - \bar{A}_e C_e T_e = \bar{A} C T = q, \quad (3.102)$$

where \bar{A}_b and \bar{A}_e are submatrices of the complete $m \times n$ matrix \bar{A} of connections of all circuit nodes and branches that fix separately the initial “ b ” and the final “ e ” nodes of the branches; $C_b = [c_{bi}]$ and $C_e = [c_{ei}]$ are diagonal matrices of the heat capacity magnitudes of the medium flowing to the initial node of branch i (c_{bi}) and out of the final node of the same branch (c_{ei}); $C = [c]$ is a diagonal matrix of the average heat capacities of flows; T_b , T_e , and T are vectors of the temperatures at the initial and the final nodes and on the circuit branches, respectively; and q is a vector of external heat sources and sinks at the circuit nodes.

When adjusting ρ_i , we determine the density $\rho_{i\theta}$ of every θ th component of the i th flow from the thermodynamic equation of state, and calculate the total flow density by the relation

$$\rho_i = \frac{\sum_{\theta} \rho_{\theta i} x_{\theta}}{\sum_{\theta} x_{\theta}}, \quad (3.103)$$

where x_{θ} is the mole quantity of the θ th component.

At the second and following iterations, system (3.6)–(3.8) is calculated with the adjusted values of H_g and ρ . In this case, if for some branch, T_i happens to exceed the ignition temperature T_{fi} of the moving medium, the flame characteristics for it are determined by MEIS (or the stoichiometric model) and then the circuit parameters are adjusted by the algorithm applied at the first iteration. The calculations terminate, if the difference in the values of x_i (or some other variables) at two successive iterations does not exceed a given small value ε .

If the model of fires is constructed on the basis of the method of nodal potentials, equation (3.93) is replaced by the expression

$$h - H_g = \bar{A}^T \bar{P}(x). \quad (3.104)$$

The closing relation for each branch with a nonzero difference of geodetic mark level z_i includes the term

$$H_{gi} = z_i \rho_i. \quad (3.105)$$

It is evident that description of the gravitational heads on the branches by relation (3.105) in the “potential” model is mathematically equivalent to description of the gravitational heads in the loops when the loop system of equations is used.

Of course, relation (3.105) may also be used to describe fires on the basis of the extreme model (3.50)–(3.56), which can obviously be reduced, as well model (3.92)–(3.97), to the model with lumped, iteratively corrected parameters. With system (3.50)–(3.56) the principle of extreme description of hydraulic systems is realized most successively: The MEIS is applied both to the search for the extreme concentration x^{ext} of harmful substances and for the maximum entropy for a closed active circuit.

Note that application of model (3.50)–(3.56) supposes a transformation of the initial calculated scheme of the air exchange system that is similar to the one presented in Fig. 3.7*b*. The variant of “extreme” description of fire is also possible on the basis of the model of an open heterogeneous circuit and choice of the corresponding objective function.

Fig. 3.8 illustrates the modeling of the system of combustion and removal of harmful industrial waste. Here branches 2–5, 3–4, 7–10, and 8–9 model devices in which the combustion process takes place, and branches 1–2, 2–3, 4–5, 5–6, 6–7, 7–8, 9–10, and 1–10 are the incoming and outgoing pipelines. Air is supplied to node 1, products of harmful substance combustion are removed from node 6. Inflows to nodes 2, 3, 9, 10 represent the burnt harmful waste.

The iterative computational process can be represented in a fashion similar to the process considered above, where the model of fires was discussed. At the first iteration the flow distribution is calculated on the assuming that no chemical reactions exist. Closeness of the pressure to atmospheric pressure and its negligible change allow one to take density of the moving medium to be constant and to use

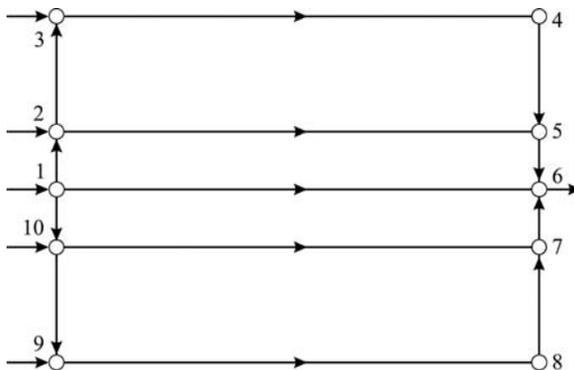


FIGURE 3.8. Hydraulic circuit of the system for removal of harmful industrial waste.

the circuit with lumped parameters. The MEIS-based information on the flow of air and harmful substances through the combustion devices is applied to calculate a combustion process and to adjust density of the moving medium on branches 2–5, 3–4, 7–10, 8–9, 4–5, and 7–8; then, according to the rules of flows mixing, the same is done on branches 5–6 and 6–7. Further, the calculations are repeated iteratively, until the differences in values of the vector x components at a transition from the k th to the $(k + 1)$ th iteration become lower than the given small value ε . From the result of the computational process it can be determined, for example, if the products of incomplete combustion are formed at individual combustion devices because of air shortage, and if incomplete combustion leads to appearance of explosive mixtures in the outgoing pipelines.