Thermodynamics and construction of physical-mathematical and technical-economic models of energy systems and technologies

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Models of energy systems, which are constructed to solve topical problems, are normally versatile and include optimization of physical–technical, technical-economic and social parameters. There are illustrative examples of combining physical and economic variables within a single analysis. Moreover, modeling of physical systems by means of thermodynamics has important theoretical achievements which may turn out to be extremely useful when generalized for economic and social systems. In particular, the possibility of replacing the dynamic description of economic systems by the analysis of a series of rest states which provides tangible advantages is shown[1].

Key words: **equilibrium thermodynamics, modeling of energy systems, modeling technology.**

Control of operation and development in the energy sector, unlike any other sector of the economy, combines physical, technical, economic, environmental and social problems, as well as energy supply reliability and security issues. This interweaving is explained by a great diversity of components that constitute energy, schemes of their relations, conditions for their interaction and operation principles. The versatile nature of the problems is determined by an interdisciplinary character of energy research, the need to create a theoretical foundation for construction of mathematical models to provide a single language for interpreting physics, engineering, economics and sociology.

Construction of such models is particularly important for analysis of energy problems in the Eastern regions of Russia. This is explained by many factors: a huge territory, a severe climate, which requires large investments in heat supply; a great number of areas with inadmissibly polluted nature, which is so vulnerable here; and a quality of life, which is considerably lower than in the central regions of the country. Aggravation of the environmental problems is caused to a great extent by construction of numerous chemical, metallurgical and other energy-intensive enterprises sited in the areas with “cheap” hydro energy. Creation of the powerful industrial complexes utilizing this energy did not take into account environmental and social problems. The one-sided analysis of the kind can not be allowed in solving the problems of developing energy export to the neighboring Asian countries, which will additionally exacerbate the current situation.

Creating interdisciplinary, multi-aspect models, it is undoubtedly necessary to use great experience of formalization which has been accumulated in physics in the analysis of a great variety of phenomena. To our mind the opinion on inapplicability of physics to economics, that sounds sometimes, is erroneous. The economists have been using physics since long ago. As a matter of fact, the source of differential and variational calculus as well as mathematical programming, whose language is often used to describe economic problems, is physics[2]. Therefore, for correct application of these areas of mathematics it is necessary to know the preconditions implied by physicists when creating them. The mathematical economics created by L.Walras [2] rests on the theory of economic equilibrium, that was constructed by analogy with Lagrangian mechanics.

Apparently from physics it is first of all necessary to use the principles, models and methods of thermodynamics. Why thermodynamics? Because thermodynamics is the science of

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[2] Mathematical features of the problem of search for extreme, equilibrium states, which is a subject of mathematical programming, were revealed by Lagrange [1] in the analysis of conditions for equilibrium of mechanical system.

the most general regularities of the macroscopic world. Its basic principles of: conservation, equilibrium, extremality, and evolution (the second law) extend to physical, biological and social forms of matter motion. These principles are statistically substantiated (statistical mechanics was created by Gibbs for such substantiation). Similar substantiations are also applicable in the analysis of both technical and economic systems. Out of thermodynamic principles, first of all, its second law is related to the main problems of physical-technical-economic modeling.

The second law of thermodynamics can be used to determine potential directions in which the studied systems can move, for example, towards economical state that meets the environmental and reliability requirements or, on the contrary, towards uneconomical, inadmissible in terms of environment, and dangerous state. To determine this, of course, the mathematical model applied should include a thermodynamic function, i.e. entropy. Entropy is a measure of probability, chaos and disorganization of state. It changes in the isolated systems according to the second law of thermodynamics only towards increase, a motion to the point of maximum value (the point of finite equilibrium). In the analysis of physical characteristics of modeled systems the entropy (production) rise should be related to dissipation of physical energy, while in the analysis of economic problems – to dissipation, useless utilization, of economic energy, i.e. capital, money. To study the processes of self-organization (increase in degree of order) the studied object should be represented by an open system exchanging energy, matter and different resources with the environment. Based on the conditions of this system interaction with the environment it is possible to determine its thermodynamic characteristic function tending towards the minimum value which corresponds to the maximum possible level of order.

In the second half of the 20th century some experience was gained beyond the physical-chemical area of the studies. The analysis of self-organization processes in the economic and social systems was made by using different variants of non-equilibrium (irreversible) thermodynamics [3-6] and synergy [7]. The non-equilibrium modeling brought interesting theoretical results that explain the capabilities and mechanism of ordering as applied to different conditions of system development.

At the same time in the course of non-equilibrium modeling the opinion gained currency that the evolution processes accompanied by changes in the level of order can be described exclusively by non-equilibrium models and self-organization can occur only in non-equilibrium systems. The authors of the present paper, using the 25-year experience of studies on the basis of the model of extreme intermediate states (MEIS) that was developed at Energy Systems Institute have come to the conclusion that the analysis of evolution of physical-technical-economic systems can be made by applying both non-equilibrium approaches and classical equilibrium thermodynamics based on which the MEIS was constructed [8-10]. A distinguishing feature of MEIS is the use of mathematical programming (MP) (the mathematical theory of equilibria and extrema) as a language for problem description. This language turned out to be quite suitable to describe interdisciplinary problems. For example, when choosing some economic indicators as an objective function ("a subjective criterion of order" [11]) the requirements of environmental efficiency, reliability and security of the modeled system are specified as a system of constraints.

The efficiency of MEIS was tested in the studies of fuel processing and combustion processes (search for the maximal output of useful products and minimal yield of harmful ones); pollution of the atmosphere by man-made emissions (determination of maximal concentrations of pollutants); and problems of the theory of hydraulic circuits (THC) [12]: calculation of hydraulic conditions and optimal synthesis (choice of optimal schemes and parameters). Analysis of the pointed out examples revealed the possibilities of equilibrium modeling of the principally irreversible processes (motion of viscous liquid, irreversible chemical reactions, heat and mass exchange in chemical reactors), the processes of self-organization, for example, transition of chemical system to the state with the minimal content of pollutants and hydraulic system – to the state that corresponds to the least consumption of energy and economic resources and the presence of flow conditions in the branches, that differ in the level of organization (laminar and turbulent).

Certainly, improvement of MEIS and its use to solve increasingly complex problems inevitably required development of equilibrium thermodynamics principles, theoretical substantiation of admissible regions of its application and competitiveness with non-equilibrium thermodynamics, the theory of dynamic systems and other theories of trajectories (evolution). Dynamic interpretation of equilibrium state became a novelty in the analysis of equilibrium thermodynamics. Whereas in the technical and chemical thermodynamics textbooks equilibria are normally explained as the states of rest (absence of macroscopic differences of potentials and flows), the MEIS is based on the assumption which is consistent with Galileo’s relativity principle and the third law of Newton that equilibrium is the equality of action and counteraction on any infinitesimal period of time for reversible, irreversible, stationary and nonstationary processes. With such a definition of equilibrium work, heat and flows of matter can be represented as the functions of state (this was already done by Lagrange for work [1]).

For equilibrium infinitesimal periods of time it turned out impossible to establish mathematical relations among the main principles of conservative and dissipative systems: the principle of least action, the second law of thermodynamics, the theory of Onsager-Prigozhin, etc. The unsuccessful efforts to reveal such relations for finite periods of time were made by the classics of physics: Clausius, Helmholtz, Boltzmann, J. Thomson, etc. [13]. The authors of the paper made a single derivation of the mentioned regularities [14] so far only for the THC problems in which the dynamic variable – a fluid flow – was assumed as the main function of state. Obviously, the derivation of the kind can be extended to the models with conditional flows that reflect the amounts of substances involved at individual stages of the total physical-chemical mechanism of the modeled process [8-10]. Identification of interrelations between the laws of trajectories and states facilitates solving the problem of physical science that was formulated by J. Thomson and aims to explain natural phenomena by the properties of matter in motion [15].

Establishment of the mentioned interrelations only for infinitesimal periods of time is sufficient to explain the possibility of equilibrium modeling of evolution since the notion of trajectory is not used when MEIS is applied, and possible results of the processes are sought on the invariant diversity (a set of attainable states), on which any admissible trajectory that runs through any point, totally belongs to this diversity. Therefore, there is no need to know the sequence of states to be passed through in the actual process and respective equations of motion. Moving towards the sought state one can pass from point to point and meet only the condition of monotony of characteristic function. This circumstance to some extent reminds of the quant mechanics principle in which the trajectories of processes are not determined.

Simplicity and universality of the initial precondition of equilibrium thermodynamics and the absence of necessity to know kinetic equation determine the computational advantages of MEIS as compared to the “trajectory models”. These advantages certainly do not deny the need to use kinetics which will always be an important tool for calculation of speeds and duration of processes, and identification of specific features of kinetic equations.

The first physical-technical-economic MEIS [10] was created to solve the problem of optimal synthesis of hydraulic (pipeline) systems. Here the ideas of interdisciplinary modeling, that were put forward by the founder of the theory of hydraulic circuits V.Ya. Khasilev, found wide application [12,16]. In [16] on the basis of hydraulic relationship between head loss and fluid flow rate in pipe he determined the mathematical features of problems concerning the choice of optimal schemes of circuits and diagrams of head losses in individual branches. Khasilev showed the concavity of the economic cost function along the axis of flow rates and the convexity - along the axis of heads; an extraordinary flatness of this function along the axis of heads in the vicinity of extremum point; independence of relative deviation of economic cost characteristics of a system from the extremum point from such technical-economic parameters as specific cost of electricity used to pump the fluid, specific capital investments in the pipeline of various diameters, depreciation charges and maintenance costs, etc. It is clear that these parameters determine absolute values of costs and their changes when choosing non-optimal head losses. However, the shape of curves, that reflect the relationships between economic functions and technical decisions made, is determined exclusively by the equation that relates head losses and flow rates.

The MEIS of non-isolated system, which is based on the presented principles and the multi-loop optimization method applied in the THC [17] (it is assumed that the pipeline system always exchanges energy and in many cases fluid flows with the environment) has the form:

Find:

$$\min\left[F(x,P^{\mathrm{br}},P^{\mathrm{mov}})=\sum_i F_i(x_i(x),P_i^{\mathrm{br}})\right]=$$
$$=F(x^{\mathrm{ext}},P^{\mathrm{br\,ext}}) \qquad (1)$$

subject to

$$Ax=Q, \qquad (2)$$

$$\sum_{i=1}^{n}P_i^{\mathrm{mov}}x_i-\sum_{i=1}^{n}P_i^{\mathrm{br}}x_i=0, \qquad (3)$$

$$D_t(y)=\left\{x:\left|\begin{array}{c}x\le y,\\ \varphi_r(x)\le\psi_r,\ r\in R^{\mathrm{lim}},\end{array}\right.\right\} \qquad \begin{array}{c}(4)\\(5)\end{array}$$

$$P_i^{\mathrm{br}}=\mathrm{z}_i x_i^{\beta}\ ,\quad i=1,\ldots,n. \qquad (6)$$

$$F_i=a_i x_i(x)P_i^{\mathrm{br}}+b_{\mathrm{i}}x_i^{\theta_i}(x)/(P_i^{\mathrm{br}})^{\tau_i}+c_i, \qquad (7)$$

where F and F_i – cost (economic) characteristics of the entire circuit and its i-th branch; x and x_i - vector of flows and its i-th component; P^{br} and P_i^{br} – vector and its i-th component of head losses in branches; A – matrix of connections of independent nodes and branches; Q – vector of sources and sinks at nodes, P^{mov} – moving pressure in branch, which is created by a pump (compressor, fan); y – vector of flows in the initial (initial for calculations) state of the system; $D_{\mathrm{t}}(y)$ – a set of attainable states from y; φ_r and ψ_r – function of the r-th component of x, to be limited according to reliability, environment or some other conditions, and its limiting value; R^{lim} – a set of indices of uneconomic constraints; z_r – coefficient of resistance of the i-th branch; β_i – exponent that can vary in the range from unit to two; a and b – constant coefficients; θ_i and τ_i – exponents depending on the value of β_i; c_i – constant part of costs in the i-th branch.

Equations (2) and (3) determine material and energy balances. Sign «$\le$» in inequality (4) has a thermodynamic sense: $x\le y$, if it is possible to pass from y to x along a continuous trajectory along which the characteristic thermodynamic function monotonously does not increase. The inequalities of form (5) are used to formulate uneconomic requirements to the solution sought. Equality (6) is a hydrodynamic relationship between head loss and flow rate for the i-th branch, which largely determines the mathematical features of the problem solved (see above). In equation (7), that determines the economic characteristics of the i-th branch the first term in its right side represents the costs of fluid transportation, the second – the costs that are proportional to capital investments depending on the pipeline diameters and the third – the costs that do not depend on x_i and P_i^{br}.

The algorithm intended to choose the optimal variant of the pipeline system on the basis of model (1)-(7) is considerably modified as compared to the method of multi-loop optimization. In the latter the redundant closed-loop circuit and the maximum diameters (in the available set) in all branches are set as initial approximation. For the specified circuit and diameters the flow distribution among branches is determined on the basis of Kirchhoff laws.

Then by introducing fictitious sinks the closed-loop circuit is replaced by a tree for which the diameters are chosen by the method of dynamic programming. Calculations of flow distribution and diameters are iteratively repeated. During iterations the branches in which the flows appear to be negligibly small are removed. The calculation stops when the difference in the objective function values for two successive iterations turns out to be lower than the specified negligibly small value. In the algorithm implementing model (1)-(7) the flow distribution calculation on the basis of Kirchhoff laws is replaced by determination of entropy extremum, and uneconomic constraints of form (5) are added. In the determination of flow distribution the entropy extremum may turn out to be both a maximum (for active circuits) and a minimum (for passive circuits). However, the economic entropy related to the non-optimal money spending in each iteration that includes the choice of both flows and diameters will certainly decrease, i.e. inequality (4) holds true. This provides convergence of the computational process.

The method of multi-loop optimization has already found wide application in the optimization of heat-, oil-, water- and gas supply [12, 17]. The changes made can not deteriorate its convergence but increase essentially the capabilities to take into account uneconomic factors. This is facilitated not only by introduction of constraint (5) but also by transition to an extremum-based approach in the flow distribution analysis. The extremum-based approach, being almost insensitive to changes in the space of variables, enables the requirements to regulation of flow rates and heads in the circuit branches and at nodes, flow conditions, etc. to be taken into consideration during analysis. The model similar to (1)-(7) can apparently be created to deal with electric power systems and electric networks as well.

The models of extreme intermediate states of physical-chemical systems that do not include economic relationships were used at Energy Systems Institute to develop a technique for forecasting energy technologies [18]. The technique was intended to substantiate the areas of research and development works, and was based on the staged application of three types of mathematical models. The models of the first type (mainly MEIS) had to be used to determine limiting energy (efficiency, specific fuel consumption) and environmental (extreme yields of harmful substances) characteristics of physical-chemical processes. The models of the second type were supposed to be applied to estimate technical and economic parameters of energy plants on the basis of data obtained at the first stage of forecasting. The third type of models was developed to choose the optimal structures of technologies in energy systems of various scales.

Multifactor studies that include technical and economic optimization of schemes, parameters and conditions of heat supply system operation with regard to the environment and reliability requirements are conducted at the Energy Systems Institute, SB of RAS, by A.M.Kler and his colleagues. The studies are a continuation of the work started by G.B.Levental and L.S.Popyrin [12]. In these studies thermodynamics is successfully used along with hydrodynamics, theory of heat and mass transfer, chemical kinetics and other disciplines.

The proposed scheme of forecasting and to the greatest extent MEIS that was included in the scheme found wide application in the national and international projects devoted to the development of energy technologies. Implementation of these projects revealed the abovementioned efficiency of interdisciplinary modeling, in particular, MEIS. The most impressive results obtained include the thermodynamic analysis capabilities in the search for environmental characteristics of fuel combustion and processing; the use of thermodynamics in chemistry of atmosphere, which was considered impossible; equilibrium modeling of viscous liquid motion and other irreversible processes and self-organization phenomena.

The presented results of thermodynamic modeling in the interdisciplinary energy studies provide evidence that the experience gained during the studies should be actively used, and in particular, for solving the problems of energy development in the Eastern regions of Russia.

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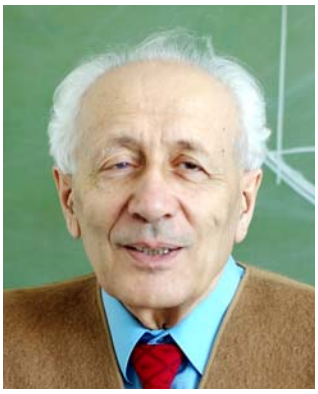

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