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Modelling non-equilibrium thermodynamic systems from the speed-gradient principle

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The application of the speed-gradient (SG) principle to the non-equilibrium distribution systems far away from thermodynamic equilibrium is investigated. The options for applying the SG principle to describe the non-equilibrium transport processes in real-world environments are discussed. Investigation of a non-equilibrium system's evolution at different scale levels via the SG principle allows for a fresh look at the thermodynamics problems associated with the behaviour of the system entropy. Generalized dynamic equations for finite and infinite number of constraints are proposed. It is shown that the stationary solution to the equations, resulting from the SG principle, entirely coincides with the locally equilibrium distribution function obtained by Zubarev. A new approach to describe time evolution of systems far from equilibrium is proposed based on application of the SG principle at the intermediate scale level of the system's internal structure. The problem of the high-rate shear flow of viscous fluid near the rigid plane plate is discussed. It is shown that the SG principle allows closed mathematical models of non-equilibrium processes to be constructed.

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1. Introduction

Questions of evolution in nature and society give rise to many different discussions where the notion of entropy is a key concept which forms the basis of modern statistical physics and thermodynamics.

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The maximum entropy principle (MaxEnt) is often used to describe the evolution of non-stationary processes. This principle states that the system that is in 'natural' conditions (in the absence of deliberate external action) tends to the state corresponding to the maximum value of its entropy. In the study of the evolution of systems, the MaxEnt allows for some cases to obtain missing information and determine the choice of mode.

The principle was first described by physicist Jaynes [1–3]. It is a simple and easy way to build statistical thermodynamics (classical and quantum), which is devoid of some difficulties, such as, for example, the ergodic hypothesis [1–4]. An important advantage of the Jaynes formalism is its ability to generalize the study of non-equilibrium systems. There are various areas of its use in the literature, including the description of relaxation processes (related to the thermodynamics of irreversible processes, Green–Kubo formulae, etc.) [1,3,5,6] and non-equilibrium phase transitions [7].

The MaxEnt is widely used in various studies of complex systems of physical, chemical and biological origin [8]. However, the issue of withdrawal of this principle has remained valid until now. This withdrawal determines how and at what trajectory the system tends to a state of maximum entropy.

It is known that the methods of optimal control such as Bellman dynamic programming, maximum principle of Pontryagin, etc., can be effectively used for modelling the dynamics of mechanical [9], thermodynamic [10] and other complex systems. For example, according to the works of Rosenbrock [11,12], the derivation of the basic equations of quantum mechanics can be obtained based on the principles of optimal control, because the Schrödinger equation is a direct consequence of the principle of optimality of the Hamilton–Jacobi–Bellman. In the context of the MaxEnt principle, the usage of optimal control methods also seems to be promising. The equations of dynamics of physical systems can be built based on the extreme principles in the case when it is possible to introduce the concept of a goal as the achievement of the objective functional extremum. As the goal, we can consider the maximization of entropy of the system and use the principle of speed gradient (SG principle) [13–17], designed to address problems of control of time-continuous systems where the above-mentioned goal is given.

The extreme SG principle has been successfully applied to construct equations of statistical dynamics of finite systems of particles that obey the principle of maximum entropy [13,18]. In [16], the experimental verification of the SG principle applicability is performed on the example of a system of particles, modelled by molecular dynamics based on the equations of classical mechanics. The dynamics of discrete systems for the Tsallis entropy is discussed in [19]. Rényi entropy is investigated from the SG principle perspective in [20]. Continuous probability distributions are considered in [21,22].

The paper deals with the application of the SG principle to the non-equilibrium distribution systems far away from thermodynamic equilibrium. We propose a new approach to describe time evolution of the system at intermediate-scale level of the system's internal structure. We show that the stationary solution to the equations, resulted from the SG principle, entirely coincides with the locally equilibrium distribution function obtained by Zubarev [4,7]. We derive new generalized dynamic equations for finite and infinite number of constraints, and also discuss the problem of the high-rate shear flow of viscous fluid near the rigid plane plate.

The problem of describing the high-speed processes in a real-world environment is very relevant in relation to the development of new technologies and devices (high-speed machines, laser technology, nanotechnology, biotechnology, medical devices, etc.). Application of the SG principle to describe processes in distributed systems far from the thermodynamic equilibrium often requires going beyond traditional models of mechanics.

In the second half of the last century, Zubarev [4,7] used the MaxEnt principle to derive the most general distribution function describing processes far from equilibrium. Following Jaynes, he was the first who incorporated all the history of macroscopic fields in the system volume into the macroscopic constraints, imposed on the system. According to the more recent papers [1,2] in which the information aspects of the Jaynes approach using the MaxEnt principle were considered, the information, included into the imposed constraints, determines the predictive

ability of the mathematical model of the system evolution. The macroscopic information used by Zubarev in his integral constraints is the most full macroscopic information about the system. It means that his distribution function is the most general and can describe macroscopic evolution of the system in the widest range of conditions far from equilibrium. Zubarev's non-equilibrium distribution function results in the integral thermodynamic relationships between the macroscopic gradients and conjugated fluxes that take into account spatio-temporal correlations and generalize the linear thermodynamic relationships of irreversible processes to high-rate and high-gradient processes. However, the generalized description is also incomplete because the explicit form of the spatio-temporal correlation functions is unknown. For many years, this was an obstacle to their use in practical problems for making the set of macroscopic transport equations complete.

To overcome these difficulties and to develop macroscopic description of non-equilibrium processes outside the framework of the conventional hydrodynamic stage close to the local equilibrium, a new approach based on the integral thermodynamic relationships is proposed [23–26]. Unlike the papers [1–4,7], where the problem of the irreversibility is considered at two-scale levels (macroscopic and microscopic), a third-scale level, intermediate between macroscopic and microscopic levels, is introduced. The new level, called mesoscopic, is determined by the first moments of the spatio-temporal correlation function in the generalized thermodynamic relationships obtained by Zubarev. As shown in papers [23–26], the spatial moments are connected to the size of new internal structure of the system and the temporal ones correspond to the living time of the structure. Experimental data [27] show that the external action, deflecting the system state far from equilibrium, gives rise to self-organization making the system structured. For example, even in homogeneous metal, as in turbulent flow of fluid, after the shock loading a formation of rotational structures of mesoscopic size was observed [28].

In this paper, we propose to move from the microscopic description of the time evolution (at which we cannot set the initial condition for the distribution function in the differential equation based on SG-algorithm) to another, mesoscopic, level of the system's internal structure. Unlike the conventional macroscopic stage of evolution valid near the local equilibrium state, the transition to the time evolution of the system's internal structure allows construction of a much more general description as far from equilibrium as we can measure the characteristics of the system's internal structure. The application of the SG principle at the mesoscopic level of the internal structure allows a prediction of the further structure evolution in the direction of maximal information entropy beginning from the measured structure. According to the SG principle, the structure evolution proceeds at a maximal rate and decays near the local equilibrium state. For the structured system, the full entropy production is always less than for the homogeneous system. Finally, the information entropy attains its maximum only in equilibrium. So, the structure formation is caused by the loss of correlation between the initial and finite microstates of the system during its evolution in the direction of the information entropy maximization under macroscopic constrains.

Investigation of a non-equilibrium system's evolution on different scale levels via the SG principle allows for a fresh look at the thermodynamics problems associated with the behavior of the system entropy. Each of the scale levels is characterized by its objective (goal) function and time needed to achieve the goal. This makes it possible to resolve some of the controversy surrounding the use of the Prigogine theorem on the minimum entropy production in the steady state of a weakly non-equilibrium system [29] and the principle of Ziegler (maximum entropy production principle (MEPP)) [30] away from equilibrium, which are implemented at different time scales. The SG principle combines the global goal of evolution: the desire to establish a steady state with a minimum of entropy losses by the fastest possible way and with the maximum entropy production at any given time, which gradually decreases as it reaches a steady state. This universality allows the SG principle to build a closed mathematical model of non-equilibrium processes with feedback between the evolution of the internal structure of the system and its macroscopic response to an external perturbation.

The approach based on the results of Zubarev and the SG principle is investigated in [23–26]. Applying this approach to the description of the shock-wave transient processes in condensed matter showed that it can be used to describe some of the detected anomalous effects, which do not find their explanation in the framework of traditional mechanical models [31–33]. As an example, in the paper the SG principle is applied to the well-known problem of mechanics, the Rayleigh problem [34] on the time evolution of the shear medium flow along the plane rigid surface. It is shown that the motion of the structureless medium is described by the SG-algorithm with the integral entropy production as a goal function and the medium velocity as control parameter. To choose another control parameter, the width of the viscous boundary layer near the surface characterizing the macroscopic structure of the flow, its time evolution is also described by the SG-algorithm. The generalized description of the time evolution at mesoscale based on the model spatial correlation function with the internal structure parameters in accordance with the SG principle shows that at a high rate the flow tends to the regime with turbulent mesoscale structure.

2. The principle of maximum entropy by Jaynes

The approach proposed by Jaynes [1–3] has become the basis for building the foundations of statistical physics based on information entropy. We present its main ideas.

Let $p(x)$ be a multivariate distribution function of the random variable. This function is unknown and it has to be defined on the basis of the information available on this system. Let us assume that we have information about some average values $\bar{H}_m$

$$\bar{H}_m = \int H_m(x)p(x)\,\mathrm{d}x, \quad m = 1, \ldots, M. \tag{2.1}$$

For the density function, it is true that

$$\int p(x)\,\mathrm{d}x = 1. \tag{2.2}$$

In general, the conditions (2.1) and (2.2) may not be sufficient for a finding of $p(x)$. In this case, according to Jaynes, the most objective way to determine the distribution function is to maximize the information entropy S_I

$$S_\mathrm{I} = -\int p(x)\log(p(x))\,\mathrm{d}x.$$

The search of maximum for S_I with additional conditions (2.1) and (2.2) is performed by means of Lagrange multipliers λ_m and leads to the following results:

$$p(x) = \frac{1}{Z}\exp\left(\sum_{m=1}^{M}\lambda_m H_m\right) \tag{2.3}$$

and

$$Z = \int \exp\left(-\sum_{m=1}^{M}\lambda_m H_m\right)\mathrm{d}x, \tag{2.4}$$

where the parameters λ_m can be determined from the conditions (2.1).

These formulae enable us to find the distribution function for the microcanonical, canonical and other ensembles, using as a (2.1) the conditions that characterize each of these equilibrium ensembles (e.g. [2,4]). It also shows that in the case of equilibrium with an appropriate choice of the random variables x, the maximum information entropy coincides with the Gibbs entropy and can be identified with the thermodynamic entropy.

Jaynes showed a deep connection and continuity of his approach to the classical works like Bernoulli and Laplace on the theory of probability and statistics, as well as the works on physics and information theory (especially J. Gibbs and C. Shannon) [3].

Although information theory initially was created with the help of concepts of statistical physics, at present, according to Jaynes, we can take the information approach as the basis for

the construction of statistical physics. According to [8], the formalism of statistical mechanics becomes a certain sequence of actions, following which we are able to get the best possible and objective assessment under significant limitations of our knowledge of the microcosm (i.e. a statistical technique to prevent possible errors).

3. Maximizing the entropy by the SG principle

The SG principle determines the law under which the system will evolve. The resulting equation for transient (non-stationary) states characterizes the dynamics of the system operation.

In accordance with the second law of thermodynamics and the Gibbs–Jaynes MaxEnt principle [2], the entropy of any physical system tends to increase as long as it does not reach its maximum possible value at the limitations imposed by other physical laws. This statement defines the asymptotic behaviour of the system for $t \to \infty$, but says nothing about how there is movement to asymptotic behaviour. To answer this question, we use the SG principle. The initial state and conditions for equilibrium are not enough to uniquely describe a system's dynamics in general. We consider the SG principle as a kind of evaluation from the class of possible dynamic movements.

(a) The system with a continuous distribution of states

Consider a system with a continuous distribution of the set of possible states. The probability distribution over states is characterized by continuous everywhere (except for a set of zero measure) non-negative probability density function $p(t, r)$ satisfying the condition

$$\int_{\Omega} p(t,r)\,\mathrm{d}r = 1, \tag{3.1}$$

where Ω is a compact set. The density distribution function is differentiable with respect to time t; one-dimensional, r can be a vector of finite dimension.

The system state evolves in time. We are interested in the behaviour of the system in steady state and in a transient mode. The steady state is determined by the maximum entropy principle: if nothing more about the system is known then its limiting behaviour will maximize its measure of uncertainty (entropy).

As a measure of uncertainty choose the information entropy. For the considering system, it is defined as

$$S(t) = -\int_{\Omega} p(t,r)\log(p(t,r))\,\mathrm{d}r. \tag{3.2}$$

The law of system's dynamics will be searched in the form

$$\dot{x} = u(t,r), \quad x = p(t,r). \tag{3.3}$$

We have to define the function $u(t, r)$. In accordance with the SG principle, it is required to calculate the rate of change of entropy (3.2) by virtue of (3.3), then calculate the gradient of this velocity with respect to u, and finally determine the actual control variables proportionally to the projection of gradient to the surface of limitations (3.1).

Let us introduce the Lagrange function for this constrained optimization problem as $S_\lambda = S(t) + \lambda'(\int_\Omega p(t,r)\,\mathrm{d}r - 1)$, where λ' is a Lagrange multiplier.

We have for $\dot{S}_\lambda$

$$\dot{S}_\lambda = -\int_{\Omega}\left(u\log p + u\frac{p}{p}\right)\mathrm{d}r + \lambda'\int_{\Omega} u\,\mathrm{d}r.$$

From (3.1), it follows that

$$\int_{\Omega} u(t,r)\,\mathrm{d}r = 0. \tag{3.4}$$

It implies that $\dot{S}_\lambda = -\int_\Omega u\log p\,\mathrm{d}r + \lambda'\int_\Omega u\,\mathrm{d}r$. Gradient of $\dot{S}_\lambda$ with respect to u is $\nabla_u\dot{S}_\lambda = -\nabla_u\langle\log p, u\rangle + \lambda'\nabla_u\langle u, 1\rangle$. According to the scalar product, we get $\nabla_u\dot{S}_\lambda = -\log p + \lambda'$.

The SG-law of motion takes the form $u = -\Gamma \log p(t,r) + \lambda$, where Γ is a scalar value, and Lagrange multiplier $\lambda = \Gamma\lambda'$ is selected to satisfy the constraint (3.4).

$$\int_\Omega (-\Gamma \log p(t,r) + \lambda)\,\mathrm{d}r = 0 \;\Rightarrow\; \lambda = \frac{\Gamma \int_\Omega \log p(t,r)\,\mathrm{d}r}{\mathrm{mes}(\Omega)}, \tag{3.5}$$

where $\mathrm{mes}(\Omega) = \int_\Omega 1\,\mathrm{d}r$.

The final equation of dynamics is given by

$$\dot{p} = -\Gamma \log p(t,r) + \frac{\Gamma \int_\Omega \log p(t,r)\,\mathrm{d}r}{\mathrm{mes}(\Omega)} = -\Gamma\left(\log p(t,r) - \frac{\int_\Omega \log p(t,r)\,\mathrm{d}r}{\mathrm{mes}(\Omega)}\right). \tag{3.6}$$

The physical meaning of the law (3.6) is moving along the direction of fastest growth of entropy, which corresponds to the maximum entropy production principle (MEPP) [8].

Stability of equilibrium together with the asymptotic convergence of solutions to the final distribution is shown in [21].

(b) Total energy constraint

The problems with a few constraints can be considered in the same way. The constraint (3.1) can be interpreted as the law of mass conservation of the system in the space Ω. Consider a system where the law of conservation of energy is also introduced. We consider the conservative case, when the energy does not depend on time. The new constraint can be described as

$$\int_\Omega p(t,r)h(r)\,\mathrm{d}r = E, \tag{3.7}$$

where E is the total energy of the system and $h(r)$ is the density of energy.

Consider the system

$$\dot{p} = u. \tag{3.8}$$

The problem is to find an operator u such that at any time t both of the constraints are satisfied and the target condition is true: $S(p(t,r)) \to S_{\max}$ for $t \to \infty$.

To solve this problem, we use the SG principle. As the goal function, we take

$$Q(p) = S_{\max} - S + \lambda_1'\left(\int_\Omega p(t,r)h(r)\,\mathrm{d}r - E\right) + \lambda_2'\left(\int_\Omega p(t,r)\,\mathrm{d}r - 1\right),$$

where S is a differential entropy, λ_1' and λ_2' are Lagrange multipliers.

According to the SG principle, the operator u must be taken in the form $u = -\Gamma\nabla_u\dot{Q}(p,u,t)$. We calculate the time derivative of a goal function

$$\dot{Q} = \int_\Omega u(t,r)\log p(t,r)\,\mathrm{d}r + \lambda_1'\int_\Omega u(t,r)h(r)\,\mathrm{d}r + (\lambda_2'+1)\int_\Omega u(t,r)\,\mathrm{d}r.$$

The gradient with respect to u is

$$\nabla_u\dot{Q} = \log p(t,r) + \lambda_1'h(r) + (\lambda_1'+1)u(t,r).$$

Finally,

$$u = -\Gamma \log p(t,r) + \lambda_1 h(r) + \lambda_2, \tag{3.9}$$

where $\lambda_1 = -\Gamma\lambda_1'$, $\lambda_2 = -\Gamma(\lambda_2'+1)$.

Now we find Lagrange multipliers λ_1 and λ_2 based on constraints conditions. For simplicity, we omit the arguments of functions. For example, instead of $\log p(t,r)$ we write $\log p$.

From constraint (3.4), we have

$$-\Gamma\int_{\Omega}\log p\,\mathrm{d}r+\lambda_1\int_{\Omega}h\,\mathrm{d}r+\lambda_2\,\mathrm{mes}(\Omega)=0. \tag{3.10}$$

From condition (3.7), equivalent to the expression $\int_{\Omega}uh\,\mathrm{d}r$, it follows that

$$-\Gamma\int_{\Omega}\log(p)h\,\mathrm{d}r+\lambda_1\int_{\Omega}h^2\,\mathrm{d}r+\lambda_2\int_{\Omega}h\,\mathrm{d}r. \tag{3.11}$$

Solving the system of equations (3.10) and (3.11), we obtain

$$\lambda_1=\Gamma\frac{\mathrm{mes}(\Omega)\int_{\Omega}\log(p)h\,\mathrm{d}r-\int_{\Omega}\log(p)\,\mathrm{d}r\int_{\Omega}h\,\mathrm{d}r}{\mathrm{mes}(\Omega)\int_{\Omega}h^2\,\mathrm{d}r-(\int_{\Omega}h\,\mathrm{d}r)^2} \tag{3.12}$$

and

$$\lambda_2=\Gamma\frac{\int_{\Omega}\log(p)\,\mathrm{d}r\int_{\Omega}h^2\,\mathrm{d}r-\int_{\Omega}h\,\mathrm{d}r\int_{\Omega}\log(p)h\,\mathrm{d}r}{\mathrm{mes}(\Omega)\int_{\Omega}h^2\,\mathrm{d}r-(\int_{\Omega}h\,\mathrm{d}r)^2}. \tag{3.13}$$

Equations (3.12) and (3.13) are defined when denominator in both fractions is not zero. If the Cauchy–Schwarz inequality is taken for $f=h$ and $g=1$, then we have the following inequality:

$$\left|\int_{\Omega}h\,\mathrm{d}r\right|^2\le\mathrm{mes}(\Omega)\int_{\Omega}h^2\,\mathrm{d}r. \tag{3.14}$$

This inequality becomes an equality when $h=\mathrm{const}$. This is the case when all energy levels are the same. Such cases will be regarded as degenerate and will not be considered. Thus, the expression

$$\mathrm{mes}(\Omega)\int_{\Omega}h^2\,\mathrm{d}r\neq\left(\int_{\Omega}h\,\mathrm{d}r\right)^2 \tag{3.15}$$

is always true.

Substituting (3.9) into the equation (3.8), taking into account (3.12) and (3.13) we obtain the equation of the dynamics in the following form:

$$\begin{aligned}\dot{p}(t,r)=&-\Gamma\log p(t,r)+\Gamma\frac{\mathrm{mes}(\Omega)\int_{\Omega}\log(p)h\,\mathrm{d}r-\int_{\Omega}\log(p)\,\mathrm{d}r\int_{\Omega}h\,\mathrm{d}r}{\mathrm{mes}(\Omega)\int_{\Omega}h^2\,\mathrm{d}r-(\int_{\Omega}h\,\mathrm{d}r)^2}h(r)\\&+\Gamma\frac{\int_{\Omega}\log(p)\,\mathrm{d}r\int_{\Omega}h^2\,\mathrm{d}r-\int_{\Omega}h\,\mathrm{d}r\int_{\Omega}\log(p)h\,\mathrm{d}r}{\mathrm{mes}(\Omega)\int_{\Omega}h^2\,\mathrm{d}r-(\int_{\Omega}h\,\mathrm{d}r)^2}.\end{aligned} \tag{3.16}$$

The general form of the evolution law (3.16) can be represented in an abbreviated form

$$\dot{p}=\Gamma\Psi\log p,$$

where Ψ is a linear integral operator that is independent of p.

$$\Psi=-I+\frac{(1,\cdot)}{\mathrm{mes}(\Omega)}+\frac{\tilde{h}(\tilde{h},\cdot)}{\|h\|^2-\frac{1}{\mathrm{mes}(\Omega)}(1,h)^2},$$

where I is identity operator, $\tilde{h}=h-(1/\mathrm{mes}(\Omega))\int_{\Omega}h\,\mathrm{d}r$.

4. Zubarev's method of non-equilibrium statistical operator

The macroscopic state of a non-equilibrium distributed system at time t is entirely determined if the density fields of mass, momentum and energy are given. Macroscopic densities are equal to the dynamic densities averaged over a distribution function. Following Jaynes [1–3], Zubarev [4] sought the non-equilibrium distribution function that maximized the information entropy under the conditions specifying the density fields induced in the system after a contact with its surroundings. A very complete overview of Zubarev's results together with an analysis of relations between different theories on the non-equilibrium processes description is presented in [35].

As a set of the averaged values $\langle P_m \rangle^t$ of the dynamic density operators of energy, momentum and particles number P_m is given at time t, the distribution function corresponds to the locally equilibrium statistical operator that describes the given non-equilibrium state of the system only via the macroscopic parameters

$$f_{\mathrm{loc}} = \exp\left\{-\Phi - \sum_m P_m F_m(t)\right\}. \tag{4.1}$$

Lagrange multipliers Φ, F_m have a meaning of macroscopic parameters depending on the space and time variables. The locally equilibrium statistical operator (4.1) describes thermodynamic medium properties and hydrodynamic processes in the local equilibrium state. Therefore, it cannot describe dissipative processes and irreversible system evolution. In thermodynamic equilibrium, the distribution f_{loc} is converted into the Gibbs distribution

$$f_0 = \exp\left\{-\Phi_0 - \sum_m P_m F_{0m}\right\}, \tag{4.2}$$

which not only maximizes the information entropy, but unlike (4.1) satisfies to Liouville equation. In equilibrium, the thermodynamic entropy is identical to the maximal value of the information entropy $S = \Phi_0 + \sum_m \langle P_m \rangle_0 F_{0m}$.

The index m can be assumed to take both discrete and continuous values. Then, the summation over m simultaneously denotes integration over the space coordinates. In this case, the non-local effects can be taken into account.

Irreversible processes of thermoconduction and viscous friction followed by the entropy production are due to deviations from local equilibrium. In order to describe the irreversible processes, the retardation (memory) effects should be taken into account. If to seek a distribution function maximizing the information entropy on the condition that the macroscopic densities are given not only at time t but at each instant in the interval $(\infty, t]$, then the result is the non-equilibrium statistical operator

$$f = \exp\left\{-\tilde{\Phi} - \sum_m \int_\infty^t \mathrm{d}t' \Re_m(t, t') P_m(t')\right\}, \tag{4.3}$$

where $\tilde{\Phi}, \Re_m(t, t')$ are Lagrange multipliers. Non-equilibrium distribution function (4.3) satisfies the Liouville equation with a source related to an interaction with surroundings and can describe the irreversible system evolution.

At the hydrodynamic stage of the evolution, the macroscopic densities averaged over the non-equilibrium distribution function (4.3) are identical to those averaged over the locally equilibrium function (4.1). Maximization of the information entropy in non-equilibrium process has been proven by Glansdorf & Prigogine [29] to lead to the evolution criterion. According to the criterion in a real non-equilibrium process, a part of the entropy production decreases. In the linear approximation in the thermodynamic forces, the Prigogine theorem on the minimal entropy production in a non-equilibrium stationary state [1,29] has been proven. Unlike linear thermodynamics of irreversible processes, the local entropy production $\sigma(r, t) \geq 0$ ceases being always positive and in non-equilibrium processes can change its sign. It has been shown that the non-local effects can provide at any time only the positive full entropy production $\int_{-\infty}^t \mathrm{d}t' \int \mathrm{d}r \sigma(r, t') \geq 0$. Accounting both non-local and memory effects allows only the following statement

$$S(+\infty) - S(-\infty) = \int_{-\infty}^{+\infty} \mathrm{d}t \int \mathrm{d}r \sigma(r, t) \geq 0.$$

In order to describe the system evolution, it is necessary to solve the macroscopic transport equations obtained by averaging dynamic transport equations for operators over the non-equilibrium distribution (4.3). The generalized macroscopic transport equations are integral-differential and include non-local and memory effects [4,36,37]. The usual hydrodynamic equations can be obtained in the first approximation, taking the macroscopic gradients as small

parameters. The relaxation equations are derived by expanding the generalized equations in the small differences of macroscopic densities.

5. Generalization of Zubarev's results based on the SG principle

We consider distributed system where the distribution function depends on the spatial coordinates.

(a) The generalization for a finite number of constraints

The above method of entropy maximization based on the SG principle can be generalized to an arbitrary finite number of constraints on the example of the MaxEnt principle by Jaynes.

Suppose we have a finite number M of constraints that are defined in the form (2.1).

Constraint (2.2) is also always true for the probability density function. As before, use the Lagrange method. We define the functional Q as

$$Q = S + \sum_{m=1}^{M} \lambda(m) \left[\bar{H}(m) - \int H(m,x) p(x,t)\, \mathrm{d}x \right] + \lambda_0 \left(1 - \int p(x,t)\, \mathrm{d}x \right),$$

where λ_m is Lagrange multiplier. Then, we can calculate the following values:

$$\dot{Q} = \dot{S} - \sum_{m=1}^{M} \lambda_m \int H_m(x) \dot{p}(x,t)\, \mathrm{d}x - \lambda_0 \int p(x,t)\, \mathrm{d}x$$

$$\nabla_u \dot{Q} = \nabla_u \dot{S} - \sum_{m=1}^{M} \lambda_m H_m(x) - \lambda_0$$

$$\nabla_u \dot{S} = -\log p(x,t),$$

The general equation of dynamics on the basis of the SG principle has the form

$$u = -\Gamma \left[-\log p(x,t) - \sum_{m=1}^{M} \lambda_m H_m(x) - \lambda_0 \right]$$

For the stationary case, the statement $u = 0$ is true. It means that

$$\log p(x,t) = \sum_{m=1}^{M} \lambda_m H_m(x) - \lambda_0$$

Then, we have

$$p = C * \exp\left(- \sum_{m=1}^{M} \lambda_m H_m(x) \right), \tag{5.1}$$

where $C = \exp(-\lambda_0)$.

From equation (2.2), we see that

$$C = \frac{1}{\int \exp(-\sum_{m=1}^{M} \lambda_m H_m(x)).}$$

It can be seen that equation (5.1) coincides with the equations for the distribution (2.3) and (2.4) and also corresponds to the principle of Jaynes.

(b) Generalization for an infinite number of constraints

These equations can also be extended for an infinite number of constraints. In this case, parameter m takes not only discrete but continuous values. Then, the functional Q takes the form

$$Q = S + \int_m \lambda(m)\left[\bar{H}(m) - \int H(m,x)p(x,t)\,\mathrm{d}x\right]\mathrm{d}m + \lambda_0\left(1 - \int p(x,t)\,\mathrm{d}x\right).$$

The way to derive the dynamics equation will not change. The general equation takes the form

$$u = -\Gamma\left[-\log p(x,t) - \int_m \lambda(m)H(m,x)\,\mathrm{d}m - \lambda_0\right]. \tag{5.2}$$

The final distribution can be obtained in a similar manner.

If the constrains are imposed on the averaged values of the dynamic density operators of energy, momentum and particles number, the stationary solution of the equation (5.2) entirely corresponds to the local-equilibrium distribution (4.1) obtained by Zubarev. After the local-equilibrium state is reached, and the information entropy achieved its maximum, the system evolution continues via the averaged values at the macroscopic level in the reversible way. The non-stationary solution of the equation (5.2) in the framework of the SG principle describes the irreversible system evolution in the direction of the local-equilibrium state. However, the differential equation of SG-laws requires the initial condition for the non-equilibrium distribution function which is unknown in the general case. According to hypothesis [38,39], the system forgets its initial state during the time evolution that allows a transition to the final evolution stage described by the reduced set of macroscopic variables. Zubarev tried to compensate the lack of information about the initial distribution function with the full information about the history of macroscopic evolution of the system far from equilibrium. Then the description should be the most general. However, the description, accounting of the memory and non-local effects, is also incomplete because of the unknown spatio-temporal correlation functions $\Re_m(r,r',t,t')$ in (4.3). So, a new approach is needed to develop an adequate description of the real physical processes far from equilibrium which are characterized by special features that distinguish them from the simply non-stationary ones.

6. Special features of non-equilibrium processes

Modern understanding of non-equilibrium processes in distributed systems based on experimental data, obtained with the use of high-precision instruments, is fundamentally different from the previously common opinion that non-equilibrium processes are irreversible non-stationary processes which can be described by partial differential equations [28,31,40]. Attempts to apply conventional mathematical models far from thermodynamic equilibrium led to serious errors. The main problem is that all physical concepts are at any rate related to equilibrium system states and a generalization of one concept implies the revision of all the basics. In order to avoid contradictions in the construction of mathematical models, an understanding of special features characterizing the system's reaction to an external perturbation much deflecting the system state from equilibrium is needed.

At rather large, macroscopic scale the linear laws adequately describe processes in distributed systems near local equilibrium. High-rate and rapidly occurring processes are characterized by much smaller spatio-temporal scales on which the internal structure effects appear. Experimental results, obtained in the study of non-equilibrium processes in different branches of mechanics (hydrodynamics of turbulent flows, multi-phase flows, shock-induced wave processes in solids, biomechanical processes), show many similar characteristics of the non-classical system reaction to external perturbations. Far from equilibrium processes are often followed by self-organization of new internal structures [7,28,29,31,32,40] such as boundary layers, mass velocity pulsations, vortex structures, localized inhomogeneities, etc. The observable self-organization effects are characterized not only by the medium properties (composition, phase state) but also by the loading regime, boundary conditions and the system geometry.

The system relaxation to thermodynamic equilibrium after perturbation due to the collective interaction effects is followed by the internal structure evolution that influences the macroscopic properties of the system. The rate of the structure evolution can change and lead to structure transitions with switching from one mode to another. The appearing feedback form the internal control closed-loops [23,24].

So, an adequate description of non-equilibrium processes requires to go beyond the conventional mechanics models and to develop a new approach at the intersection of statistical mechanics, theory of nonlinear integral sets and control theory.

7. Non-local thermodynamic relationships with memory

Critical analysis of the situation with the description of non-equilibrium processes allows a conclusion that the conventional differential models of physical systems are not valid for high-rate processes and strongly inhomogeneous systems. As non-equilibrium statistical mechanics shows [4,36,37,41] macroscopic transport equations far from equilibrium should be spatially non-local and contain the memory about the process history. In the general case, the description of non-equilibrium processes in terms of a distribution function is virtually unavailable. Therefore, it makes sense to describe non-equilibrium processes immediately at the macroscopic level, using the non-local hydrodynamic equations with memory.

Zubarev by the non-equilibrium statistical operator method [4] obtained the integral relationships between thermodynamic forces $G(r,t)$ (gradients of macroscopic fields) and fluxes $J(r,t)$

$$J(r,t) = k_0 \int_{-\infty}^{t} \mathrm{d}t' \int_V \mathrm{d}r' \Re(r,r',t,t') G(r',t') = \int_{-\infty}^{t} \mathrm{d}t' \int_V \mathrm{d}r' \Re(r,r',t,t') J_0(r',t'). \tag{7.1}$$

The relationships (7.1) generalize the linear and local thermodynamic relationships

$$J_0(r,t) = k_0 G(r,t) \tag{7.2}$$

(k_0 are transport coefficients) which is valid near equilibrium, to the processes far from equilibrium. The integral kernels $\Re(r,r',t,t')$ are non-equilibrium spatio-temporal correlation functions of thermodynamic fluxes which introduces nonlinear, non-local and memory effects into the system reaction. The correlation functions are nonlinear functionals of the history of macroscopic fields all over the system volume, including boundary interaction. Macroscopic expressions for the functionals are unknown in the general case.

The relationships (7.1) close the set of macroscopic transport equations on non-equilibrium conditions and make equations non-local and retarding. Instead of the distribution function the generalized equations contain more rough characteristics of non-equilibrium processes, the integral functionals of macroscopic variables. The non-local and memory effects occur as a payment for the inevitable incompleteness of description of non-equilibrium processes in open system. Despite the fact that the non-local mathematical models with memory are the only fundamentally new over the past two centuries, these results so far have not been claimed because of the problems on the correlation functions modelling and misunderstanding of the link between correlations and boundary conditions imposed on the system from outside.

8. New approach based on non-local theory of non-equilibrium transport processes

Based on the non-local and retarding relationships (7.1) obtained in non-equilibrium statistical mechanics, a new self-consistent theory of the transport processes far from equilibrium has been developed by Khantuleva and colleagues [25,26,31,40]. The new universal approach to the transition processes in open systems with internal structure evolution relies on the non-local and retarding relationships (7.1) generalized to take into account the structure effects. The first statistical moments of the correlation function have been found to characterize the

internal structure scale. The model of spatio-temporal dependence $\Re(r, r', t, t')$ constructed in correspondence with the known asymptotic limits should depend on the structure parameters s (having dimension of length) incorporated into the model,

$$J(r,t) = k_0 \int_{-\infty}^{t} \mathrm{d}t' \int_V \mathrm{d}r' \Re(r, r', t, t', s) G(r', t') = \int_{-\infty}^{t} \mathrm{d}t' \int_V \mathrm{d}r' \Re(r, r', t, t', s) J_0(r', t'). \tag{8.1}$$

For structureless continuous medium, $s \to 0$ (8.1) converts into the linear relationships (7.2). In this case, the non-local and memory effects are caused by the collective interaction and internal structure formation. The detection of a connection between the non-equilibrium correlation function and the wave-vortex internal structure was a big step forward to the nature of non-equilibrium processes. Boundary conditions imposed on the system lead to a discretization of the spectrum of the parameters s, i.e. self-organization (the structuring of the system). The result, like in quantum mechanics, corresponds to the modern tendency in mathematics to discretization connected to computer engineering. The structure parameters become nonlinear functionals of macroscopic fields and boundary conditions. The internal structure interaction generates the structure evolution with internal control described by cybernetic methods.

Only such interdisciplinary approach at the intersection of statistical mechanics, physics and cybernetics can close the self-consistent formulation of boundary problems on non-equilibrium processes in open systems and predict the system evolution and new structure formation. In papers [31–33,40], the elastic–plastic transition inside the shock-induced pulse running in solid material and followed by new structure formation at mesoscopic scale is described using the non-local theory of non-equilibrium transport. In the paper [33], the transition to quasi-stationary regime of the elastic–plastic wave propagation results from the SG-algorithm. The developed nonlinear and non-local mathematical models with memory have been found to adequately describe the experimentally observable effects and offer new possibilities for developing of modern technologies to get materials with the desired internal structure.

9. The SG principle for describing the system structure evolution

Non-equilibrium transport processes are induced in macroscopic systems under dynamic loading and are followed by the structure formation of different kind: vortexes, dynamic pulsations, near-boundary structures, etc. The structure transformation can lead to different instabilities and change the macroscopic properties of the system. It is the structure evolution during non-equilibrium process that binds the problem of the description of non-equilibrium processes and the control theory. The internal structure is the information carrier and it is by means of the structure interaction the information-control feedback is forming in the system far from equilibrium. So, the inclusion of the self-organization and internal control closed-loops are prerequisites for an adequate modelling of non-equilibrium processes.

The main question arising in the formulation of the problem in scope of the control theory concerns to the choice of a goal function and ways to achieve it. The laws governing the internal structure transformation are defined by thermodynamic principles and the energy exchange between different degrees of freedom at the internal structure scale. An evolution should have its direction determined by irreversible dissipation of mechanical energy into heat (chaotic motion at microscale) and the system relaxation to thermodynamic equilibrium characterized by maximal entropy value.

In the paper, maximization of the full entropy production in the system is chosen as a control goal (goal of the system evolution) and the SG-algorithm [13,17,18,23,24] should describe the shortest way to achieve the goal. The rates of the structure scale characteristics are chosen as the control parameters. The SG principle imbedded in the internal control mechanism of the non-equilibrium system is an engine of the system evolution. Transforming its internal structure, the system minimizes its irreversible losses and contains information about the history of the imposed external loading. According to the SG-algorithm, the system evolution is represented as a trajectory on the hypersurface constructed above the control parameters space. The phase point

should go down the trajectory bounded by the imposed conditions. If the trajectory is known, it becomes possible to predict the future reaction of the system which from the point of view of conventional approaches, based on 'rigid' models [42], seems to be unpredictable.

For the non-equilibrium processes instead of the local entropy production, used in conventional continuum mechanics, only the integral characteristics can serve for the goal formulation. In paper [43], Lucia has introduced a capacious concept of the entropy generation defined as the full entropy produced by the system all over the process history

$$\Sigma(t) = \int_0^t \mathrm{d}t \int_V \mathrm{d}x J(x,t) G(x,t). \tag{9.1}$$

Then, the integral entropy production is the rate of the entropy generation

$$\dot{\Sigma}(t) = \int_V \mathrm{d}x J(x,t) G(x,t). \tag{9.2}$$

In the region of linear thermodynamics of irreversible processes where thermodynamic fluxes are proportional to forces, (9.2) takes a form

$$\dot{\Sigma}(t) = k_0 \int_V \mathrm{d}x G^2(x,t). \tag{9.3}$$

According to the Prigogine theorem proved in linear thermodynamics, the local entropy production takes its minimal value in the stationary non-equilibrium state maintained by the imposed boundary conditions. This result should be valid for the integral entropy production too. However, far from equilibrium the result is not proved. The macroscopic system, deviated far from equilibrium, relaxes to equilibrium with maximal entropy generation and zero entropy generation rate. The system with imposed boundary conditions also relaxes to more equilibrium state with the smaller entropy generation. According to the SG principle, if it is a stationary state the evolution trajectory should go down to the plane with constant and minimal value of the entropy production rate. This entirely corresponds to the Prigogine theorem, but not bound to near equilibrium conditions. So, in the framework of the SG principle the Prigogine theorem can be generalized to nonlinear non-equilibrium processes.

Unlike the Prigogine theorem, Ziegler [8,30] argues the opposite seemingly: the system far from equilibrium tends to maximize its local entropy production. Despite claims of the Ziegler principle's validity in a wide range of non-equilibrium conditions, the local entropy production does not describe the system evolution to the goal with time. It only says that at any time during the evolution the local entropy production should be maximal, though the maximal value should be zero in the final equilibrium state.

Both seemingly opposite results can be combined in the framework of the SG principle: the goal function is defined by the maximal entropy generation and minimal entropy generation rate on the imposed boundary conditions, but the way to the goal, defined by the SG-algorithm, goes along the gradient on the surface of the entropy generation rate at maximal rate. So, the proposed formulation of the internal control problem considers being acceptable at any rate for the non-equilibrium systems which evolution is entirely defined by the internal structure evolution.

The SG-algorithm has two different forms: differential for the wave-type processes and finite for more slow relaxation. As the integral values, such as the entropy generation, change more slow than macroscopic gradients the structure evolution supposes being slow and can be described by the finite form of the SG principle. This circumstance causes separation of variables in scale that is the necessary condition for self-organization of new structures in non-equilibrium system. Only under the condition, the concept of internal structure itself is meaningful. The finite form of the SG-algorithm results in a set of nonlinear differential equations with respect to the rates of the structure parameters $\dot{s}$

$$\dot{s} = \dot{s}(t = t_0) - g \nabla_s \dot{\Sigma}. \tag{9.4}$$

Coefficient $g > 0$ is an empiric constant characterizing inertial properties of the system's internal structure. Through the entropy production rate in the right part of (9.4), the feedback

between the structure evolution and macroscopic relaxation is introduced, and the control problem formulation of the system's evolution becomes closed and self-consistent. The control closed-loops are known to make systems more stable than 'rigid' programme control.

It must be noted that the finite form of the SG principle (9.4) entirely coincides with the steepest descent algorithm with the goal (9.2) and control parameters s

$$\dot{s} = -g\nabla_{\dot{s}}\ddot{\Sigma} = -g\nabla_{\dot{s}}(\nabla_s\dot{\Sigma}\dot{s}) = -g\nabla_s\dot{\Sigma}. \tag{9.5}$$

The rate of the function (9.2) results in the evolution principle obtained by Glansdorff & Prigogine [29]

$$\ddot{\Sigma} = \nabla_s\dot{\Sigma}\dot{s} = -g(\nabla_s\dot{Z})^2 \leq 0. \tag{9.6}$$

The set of differential equations (9.4) needs initial conditions characterizing the internal structure resulting from the external action. The evolution trajectory goes down from this point on the surface (9.2). In the general case, the initial point is unknown, but in practice it is possible to calculate one of the trajectory points from experimentally measured macroscopic characteristics, solving the inverse problem with respect to the structure parameters. The approach was used in paper [33] for the elastic–plastic shock-induced wave evolution. It should be underlined that only the set of equations (9.4) allows a closed formulation of problems on non-equilibrium processes.

10. The structure stability in non-equilibrium transport

Cybernetic methods allow a new point of view at the stability of non-equilibrium systems. Often stationary macroscopic states of non-equilibrium system simultaneously lose their stability, and it is difficult to find the reason of such behaviour. In the framework of non-local theory of non-equilibrium transport the internal structure evolution can continue even in the stationary macroscopic state because the boundary conditions maintain not all degrees of freedom. As a result a part of the structure parameters relaxes decreasing the entropy production rate. When due to the positive feedback the scale of macroscopic inhomogeneity coincides with the internal structure scale, the structure transformation occurs. In such a threshold manner the system switches to another regime of evolution. Sometimes the transformation may be called catastrophic. For example, it is a fracture of solid, non-equilibrium phase transformation, etc.

The proposed non-local approach together with the SG principle allows a direct calculation of the living time for the considered internal structure type under the imposed boundary conditions taking into account feedback in between the structure evolution and the dynamic of macroscopic fields.

11. The SG principle in non-equilibrium hydrodynamic processes

One of the known test problems in hydrodynamics is Rayleigh problem having a solution in the explicit form [34]. An evolution of a shear flow of the viscous Newtonian fluid above an infinite plane rigid plate moving at a constant velocity U_0 (figure 1) is considered. The plate at $t = 0$ supposes to be instantaneously set in motion, and further the fluid in a nearby layer begins move together it.

The motion of the incompressible viscous fluid is described by a parabolic equation for the shear mass velocity u

$$\frac{\partial u}{\partial t} = v_0\frac{\partial^2 u}{\partial y^2}, \tag{11.1}$$

where v_0 is kinematic shear viscosity. Equation (11.1) describes the momentum diffusion due to the interaction between the moving plate and the initially immovable fluid. Under the given

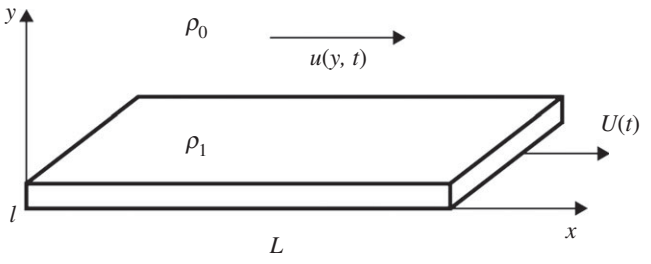

Figure 1. The flow diagram.

initial and boundary conditions,

$$u(y,t=0)=0, \quad u(y=0,t)=U_0, \quad u(y\to\infty,t)\to 0. \tag{11.2}$$

Equation (11.1) has a solution

$$u(y,t)=U_0\left(1-\mathrm{erf}\frac{y}{2\sqrt{v_0 t}}\right), \quad \mathrm{erf}(x)=\frac{2}{\pi}\int_0^x \exp -\xi^2\,\mathrm{d}\xi. \tag{11.3}$$

The velocity gradient,

$$\frac{\partial u}{\partial y}=-\frac{U_0}{\sqrt{\pi v_0 t}}\exp\left\{-\frac{y^2}{4v_0 t}\right\}, \tag{11.4}$$

is infinite at $t=0$ and decreases to zero at $t\to\infty$. Within the the linear thermodynamics of irreversible processes, the shear stress P is proportional to the normal gradient (11.4)

$$P(y,t)=v\frac{\partial u}{\partial y}=-\frac{vU_0}{\sqrt{\pi v_0 t}}\exp\left\{-\frac{y^2}{4v_0 t}\right\}. \tag{11.5}$$

Expression (11.5) has δ-singularity at $y=0,\ t\to 0$. If the initial acceleration $(\partial u/\partial t)(y,t=0)$ is finite, there is an initial regime when parabolic equation (11.1) is not valid. According to the solution (11.3), a stationary state is setting when all the fluid moves together with the plate at the velocity U_0. In the reference connected to the plate, the system state is full thermodynamic equilibrium. The local entropy production decreases with time to zero

$$\sigma(y,t)=\frac{\partial u}{\partial y}P(y,t)=v_0\left(\frac{\partial u}{\partial y}\right)^2. \tag{11.6}$$

Substitution (11.4) into (11.6) shows that σ decreases with time to zero

$$\sigma(y,t)=\frac{vU_0^2}{\pi v_0 t}\exp\left\{-\frac{y^2}{2v_0 t}\right\}_{t\to 0}\to 0. \tag{11.7}$$

The introduced above entropy generation calculated accounting (11.7), to the opposite, tends from zero to maximal value which is infinite for the infinite system

$$\Sigma(t)=\frac{U_0^2\sqrt{2v_0 t}}{\sqrt{\pi}}, \quad \Sigma(t)_{t\to\infty}\to\infty. \tag{11.8}$$

The entropy generation rate calculated for the entropy generation (11.8) tends from infinite at the initial instant to zero during relaxation

$$\dot{\Sigma}(t)=\frac{vU_0^2}{\sqrt{2\pi v_0 t}}{}_{t\to\infty}\to 0. \tag{11.9}$$

It is worth to note that equation (11.1), governing the viscous shear flow, can be derived within SG-algorithm applied to the problem under certain conditions. Choosing the entropy generation

rate (11.9) as a goal function and the fluid acceleration $\dot{u}$ as a control parameter, and using the SG-algorithm, one gets first the second time derivative of the entropy generation

$$\ddot{\Sigma}(t) = \int_0^\infty \mathrm{d}y v_0 2 \frac{\partial u}{\partial y} \frac{\partial^2 u}{\partial y \partial y} = 0 - \int_0^\infty \mathrm{d}y v_0 2 \frac{\partial^2 u}{\partial y^2} \frac{\partial u}{\partial t}.$$

Then the gradient with respect to $\dot{u}$

$$\nabla_{\dot{u}} \ddot{\Sigma}(t) = \nabla_{\dot{u}} \int_0^\infty \mathrm{d}y v_0 2 \frac{\partial^2 u}{\partial y^2} \frac{\partial u}{\partial t} = -v_0 \frac{\partial^2 u}{\partial y^2}.$$

The finite form of the SG-algorithm yields an equation

$$\dot{u} = -\Gamma \nabla_{\dot{u}} \ddot{\Sigma}(t)$$

that for the parameter value $\Gamma = 1$ on the condition $\dot{u}(y > 0, t = 0) = 0$ is identical to the momentum diffusion equation

$$\frac{\partial u}{\partial t} = \Gamma v_0 \frac{\partial^2 u}{\partial y^2}.$$

The boundary condition is not included into the system. It means that without boundary and initial conditions the equation (11.1) describes only the gradient way but not the system evolution itself. Then, the question arises: what principle the system follows during the time evolution under the conditions (11.2)?

Let an evolution parameter $\alpha(t)_{t \to 0} \to 0$ of the length dimension generates the initial δ-singularity at $y = 0, t \to 0$ in the shear stress P like $2\sqrt{v_0 t}$ in (11.5) under conditions (11.2). Then,

$$P(y,t) = v_0 \frac{\partial u}{\partial y} = -\frac{2 v_0 U_0}{\sqrt{\pi}\alpha} \exp\left\{-\frac{y^2}{\alpha^2}\right\},$$

the local entropy production within the linear thermodynamics.

$$\sigma(y,\alpha) = \frac{\partial u}{\partial y} P(y,\alpha) = v_0 \left(\frac{\partial u}{\partial y}\right)^2 = \frac{4 v_0 U_0^2}{\pi \alpha^2} \exp\left\{-\frac{2y^2}{\alpha^2}\right\},$$

the entropy generation

$$\Sigma(\alpha) = \int_0^\alpha \mathrm{d}\alpha \int_0^\infty \mathrm{d}y \sigma(y,\alpha)$$

and the entropy generation rate

$$\dot{\Sigma}(t) = \int_0^\infty \mathrm{d}y \sigma(y,t)\dot{\alpha} = \int_0^\infty \mathrm{d}y v \left(\frac{\partial u}{\partial y}\right)^2 \dot{\alpha} = \frac{2 v_0 U_0^2}{\sqrt{2\pi}\alpha} \dot{\alpha} \tag{11.10}$$

are expressed in terms of the parameter $\alpha(t)$. With the entropy generation $\Sigma(\alpha)$ in the form (11.10) chosen as a goal function and $\alpha(t)$ as a control parameter, the SG-algorithm defines an unknown temporal dependence of the parameter $\alpha(t)$

$$\dot{\alpha} = \Gamma \frac{\partial \dot{\Sigma}}{\partial \dot{\alpha}}, \quad \dot{\alpha} = \Gamma \frac{2 v_0 U_0^2}{\sqrt{2\pi}\alpha}, \tag{11.11}$$

where the constant coefficient Γ characterizes the rate of the system evolution under the given conditions. The differential equation (11.11) has a solution $\alpha^2 = \Gamma(U_0^2/\sqrt{2\pi}) 4 v_0 t$ that defines the dependence $\alpha(t) = 2\sqrt{v_0 t}$ up to a constant. It means that the temporal evolution of the shear viscous flow is going in accordance with the SG-algorithm in the direction of maximization of entropy generation.

The SG principle, as might be expected, should be valid above the limits of linear thermodynamics under much more non-equilibrium conditions.

12. Non-local generalization of Rayleigh solution to high-rate motion of the plate

High-rate motion of the plate prevents the momentum exchange between the fluid layers and the plate. The diffusive mechanism of the momentum transport has no enough time to form. As a result, wave-vortex structures are generated near the plate surface and move from it, forming the expanding with time turbulent layer. In order to describe the turbulent flow, an integral mathematical model relationship between the shear stress $P(y,t)$ and the velocity gradient, obtained in non-local theory of non-equilibrium transport processes [26], can be used

$$P(y,t) = v_0 \int_0^\infty \frac{\mathrm{d}y'}{\epsilon} \exp\left\{-\frac{\pi(y'-y-\gamma)^2}{\epsilon^2}\right\} \frac{\partial u}{\partial y'}. \tag{12.1}$$

The integral in (12.1) contains a smoothing δ-type kernel depending on parameters ϵ, γ which are tied to the size of the wave-vortex structures near the plate. The shear parameter $\gamma > 0$ introduces the boundary influence into the process model. However, for a one-dimensional problem ϵ characterizes a thickness of the layer where the fluid moves in correlation with the rigid boundary, and γ defines a rotational moment $\gamma \times u$ of the structure element near the boundary that allows the conditions (11.2) being satisfied. Big gradients near the boundary make the solution (11.3) invalid in the layer of the thickness γ and result in the mass velocity slip on the rigid surface. According to the non-local relationship (12.1), the stress is not proportional to the velocity gradient in the same spatial point at any instant, but it depends on the velocity field all over the spatial region.

In the general case, the parameters $\epsilon(t), \gamma(t)$ evolve in time and describe the wave-vortex structure evolution. Unlike the evolution of the structureless medium described by the solution (11.3), the evolution of turbulent flows goes due to the structures interaction, but not due to the momentum diffusion. Let for simplicity, an approximate model for the shear stress in turbulent flow is considered instead of (12.1)

$$P(y,t) = v_0 \int_0^\infty \frac{\mathrm{d}y'}{\epsilon} \exp\left\{-\frac{\pi(y'-y-\gamma)^2}{\epsilon^2}\right\} \frac{\partial u_0}{\partial y'}, \tag{12.2}$$

where $\partial u_0/\partial y$ is defined by (11.4).

The δ-singularity at $y = 0, t \to 0$ disappears for the finite size structures, the friction behaviour becomes inmonotoneous and decreases compared with the structureless medium at the same velocity. However, it should be recalled that the model relationship (12.1) is not correct at the initial stage of the process without the memory effects included into the model. So, it is possible to confirm only that the maximal friction value in turbulent flow should be less than in the structureless medium. The result is in accordance to one obtained by Klimontovich within the kinetic theory.

The approximate expression for the entropy generation rate with the stress (12.2) is also evolving in time

$$\begin{aligned}\dot{\Sigma}(t) &= \int_0^\infty \mathrm{d}y \sigma(y,t) = \int_0^\infty \mathrm{d}y \frac{\partial u_0}{\partial y} P(y,t) \\ &= v_0 \int_0^\infty \mathrm{d}y \frac{\partial u_0}{\partial y} \int_0^\infty \frac{\mathrm{d}y'}{\epsilon} \exp\left\{-\frac{\pi(y'-y-\gamma)^2}{\epsilon^2}\right\} \frac{\partial u_0}{\partial y'}.\end{aligned} \tag{12.3}$$

Figure 2 shows the evolution of the surface $\dot{\Sigma}(\epsilon, \gamma, u_0(t))$, constructed above the plane of the structure parameters ϵ, γ.

The maximal growth of the entropy generation rate (12.3) is localized near the origin that corresponds to the structureless fluid, described by the solution (11.3) invalid at the initial stage of the process. In course of time the surface is equalizing, as shown in figure 2. The SG principle, applied to the entropy generation rate (12.3), results in the structure evolution description.

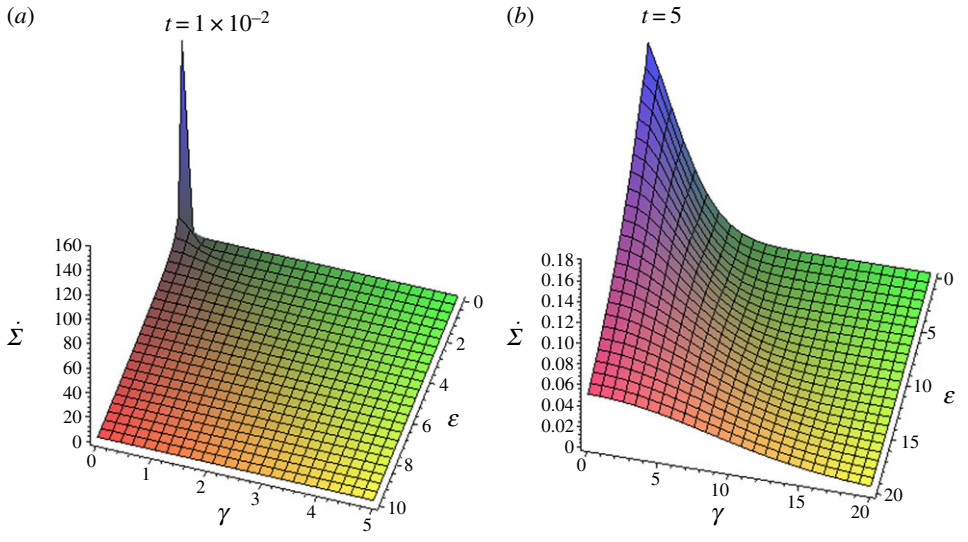

Figure 2. The surface (12.2) over the phase plane (ϵ, γ). (*a*) at instant t and (*b*) $t = 5$. (Online version in colour.)

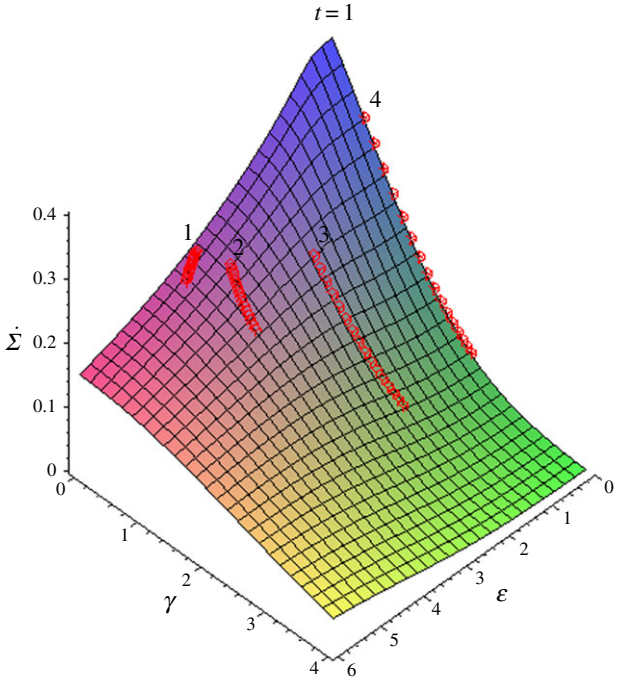

Figure 3. The SG trajectories on the surface at instant $t = 1$ going down from different initial points 1, 2, 3 and 4. (Online version in colour.)

According to (9.5), the SG-algorithm in the finite form entirely corresponds to the steepest descent algorithm with the goal (12.3) and the control parameters ϵ, γ. Figure 3 shows the structure evolution trajectories.

As shown in figure 3, the time dependence of (12.4) is non-monotonic during the evolution.

All the evolution trajectories, going down from different initial points, lead to a clusterization of the medium elements and formation of the internal medium structure. The right trajectory

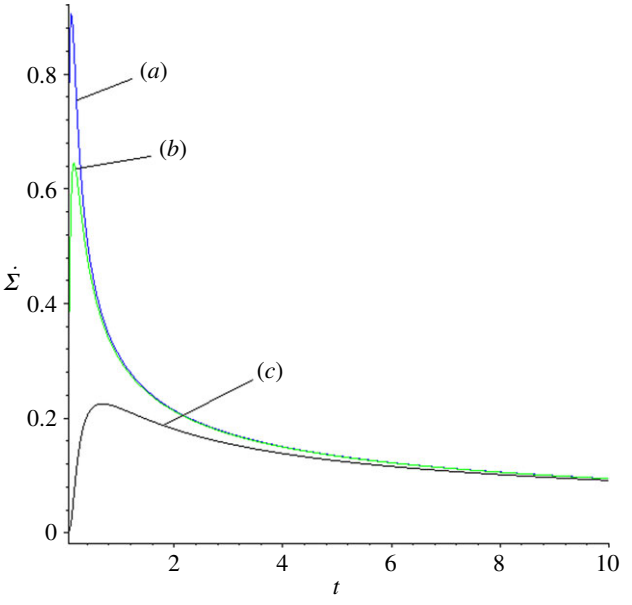

Figure 4. Time evolution of the entropy generation rate (12.4): $\gamma = 0.01$ (*a*), $\gamma = 0.2$ (*b*), $\gamma = 1$ (*c*) (in sequence downward). (Online version in colour.)

on figure 3 corresponds to the case $\epsilon \to 0, \gamma > 0$ when the entropy generation rate can be calculated.

$$\dot{\Sigma}(t) = \int_0^\infty \mathrm{d}y \sigma(y,t) = \int_0^\infty \mathrm{d}y v_0 \left(\frac{\partial u}{\partial y}\right)^2$$
$$= \frac{v_0 U_0^2}{\pi v t} \int_0^\infty \mathrm{d}y \exp\left\{-\frac{(y+\gamma)^2}{2v_0 t}\right\} = \frac{v_0 U_0^2}{\sqrt{2\pi v_0 t}} \left(1 - \exp\frac{\gamma}{\sqrt{2v_0 t}}\right). \tag{12.4}$$

Figure 4 shows that the entropy generation rate decreases due to the parameter's γ growth. The equation for the parameter $\gamma(t)$, provided by the SG-algorithm, describes the very right trajectory on figure 3.

$$\dot{\gamma} = \Gamma \frac{U_0^2}{\pi t} \exp\left\{-\frac{\gamma^2}{2vt}\right\} > 0. \tag{12.5}$$

Figure 3 shows the trajectories going down the surface fixed at one instant, but the surface itself is equalizing during the trajectories are going down. Figure 3 also shows that the entropy generation rate in the turbulent flow is always less than in the laminar one at the same high velocity of the flow. The larger the scale of the turbulent flow, the less the entropy generation rate becomes. This finding is consistent with the result obtained by Klimontovich [44], who calculated the entropy production for the turbulent gas flow using the kinetic theory.

It would be very interesting to investigate the system evolution with feedback between the changing surface of the entropy generation rate and the internal structure evolution. Boundary conditions imposed on the finite size system can originate different wave-vortex structures depending on the initial perturbations in the flow.

13. Conclusion

In this paper, it is shown that elements of the control theory are necessary to construct closed mathematical models of non-equilibrium processes which have a predictive ability. Far from

equilibrium, where the initial distribution function cannot be specified, it makes sense to leave the evolution description in terms of the distribution function and to describe the more available structure evolution. The physics of non-equilibrium processes requires the self-organization modelling, because the high-rate transport in real media is often followed by new internal structure formation at an intermediate-scale level between the macroscopic and microscopic ones [23,24,28,31,32,40]. The formed structures become the natural information carriers in the system far from equilibrium and lead to the internal closed-loops via feedback between the structural and macroscopic medium properties. So, the self-regulation, operating in accordance with the control theory principles, as shown in papers [23,24,26,31–33], is inherent not only to living systems, but, in a varying degree, to almost all material phenomena.

We consider a non-equilibrium system's evolution at different scale levels via the SG principle and show that the SG principle allows closed mathematical models for non-equilibrium processes to be constructed. We also propose a new approach to describe time evolution of a system far from equilibrium at intermediate-scale level of the system's internal structure.

Consideration of the changing structure effects requires new mathematical model (which can be called 'flexible' [42]) that change their type with time depending on the internal structure evolution. Therefore, it becomes clear that attempts to use the 'rigid' multi-parameters models, in order to describe dynamic processes within a wide range of the loading conditions, are doomed to failure.

Such 'flexible' mathematical models are constructed in the framework of the non-local theory of non-equilibrium transport processes [23–26,31,32], based on the results of non-equilibrium statistical mechanics [4,36,37,41] and methods of the cybernetic physics [14,15,18]. It is shown that the role of the SG principle in description of processes far from equilibrium becomes determinative.

The system evolution far from equilibrium, inseparably linked to the internal structure evolution, is governed by the thermodynamic goal functional, connected to the maximization of the entropy generation [43]. The fastest way to reach the goal, bounded by the imposed conditions, is described by the SG principle [14–18,21], which determines the evolution trajectories going down the moving surface of the entropy generation rate. Owing to feedback between the structure evolution and macroscopic properties of the system, this approach allows a prediction of the future system behaviour including possible turns of the trajectories.

The SG principle can eliminate the contradiction between the seemingly opposite thermodynamic principles and combine the minimal entropy production principle for stationary states, proved by Prigogine within linear theory of irreversible processes [29] and maximal entropy production in nonlinear non-equilibrium process by Ziegler [30].

We show that the control closed-loops, occurring at the internal structure level, generate new prospects for the external control, which are related to development of new technologies, intellectual systems and prediction of catastrophic processes. The set of 'flexible' mathematical models proposed in the paper provides the effective theoretical approach to solve a wide range of the modern practical problems with the use of cybernetic physics methods.

Data accessibility. All methods and corresponding data are given in the manuscript and can be fully reproducible.

Authors' contributions. T.A.K. investigated the relationship between the SG principle dynamic equations and results of D. Zubarev. D.S.S. derived generalized dynamic equations based on the SG principle and prepared the manuscript. All authors gave final approval for publication.

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