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Nonlocal hydrodynamic modeling high-rate shear processes in condensed matter

T Khantuleva¹, D Shalymov^{2,3}

¹Mathematics and Mechanics Department, St. Petersburg State University, Universitetsky pr. 28, St. Petersburg, Russia, 198504

²IPME RAS, V.O., Bolshoj pr. 61, St. Petersburg, Russia, 199178

³This work was supported by Russian Science Foundation (project 16-19-00057)
dmitry.shalymov@gmail.com

Abstract. Problem of mathematical modeling high-rate processes in condensed medium is considered by using new nonlocal hydrodynamic approach based on the results of non-equilibrium statistical mechanics and cybernetical physics. Interrelationships between the spatiotemporal correlations in the integral thermodynamic relationships between forces and fluxes and the system internal structure made it possible to describe the self-organization of new dynamic structures in the open system. The temporal structure evolution is described by methods of the control theory of adaptive systems. The proposed approach to the structure evolution allows a new insight into the system state stability. The proposed approach is used to describe high-rate shear flow in the Couette formulation. Explicit approximate solutions to the problem show that steady pure shear flow far from equilibrium loses its stability due to dynamic structure evolution. Near the boundaries there appear layers where continuum mechanics becomes invalid and non-equilibrium interfacial interaction with the walls forms vortex structures. In transient modes a meta-stable state can occur where the system evolution can change its direction due to any weak impact.

1. Introduction

The problem of a uniform description of the motions of continuous media of various nature in a wide range of modes has not been resolved up to the present time. The main difficulty lies in the choice of relations closing the transport equations beyond the applicability of generally accepted medium models. The models of non-Newtonian fluids, turbulence models are valid only in a rather narrow range of parameters, and attempts to generalize them to wider classes of problems, as a rule, lead to very cumbersome constructions that lose the physical visibility. Transient processes, such as elastic-viscous-plastic flows of deformable solids, flows with a laminar-turbulent transition, are characterized by a very complex mechanism of interaction in the medium, which can significantly depend on the integral properties of the system as a whole, on the stage of the process, on the mode of its course, on external loading conditions. Therefore, the problem of determining the limits of applicability of certain approaches and the development of a more general and universal mathematical apparatus is currently very relevant. One of the ways to solve this problem is the development of nonlocal mechanics with memory as a fundamental theory based on the rigorous results of non-equilibrium statistical mechanics, and as a flexible apparatus for solving problems, which, by virtue of its self-consistency, is also applicable in cases where the momentum mechanisms change during the process.



In the second half of the last century in non-equilibrium statistical mechanics from first principles [1,2,3] proved that far from equilibrium the correct mathematical models should be integral-differential with considering nonlocal and memory effects. To describe temporal evolution of the system out of thermodynamic equilibrium methods of the control theory of adaptive systems can be used. Lately even a new discipline of cybernetical physics [4] appeared. For the evolving physical systems far from equilibrium the feedback accounting is the necessary attribute of modeling to complete the mathematical formulation of the problem. So, it becomes clear that since for transient processes the mechanism of momentum and energy transport changes the process models out of equilibrium should not be rigid [5].

New theoretical approach to non-equilibrium momentum and energy transport [6] developed on the base of non-equilibrium statistical mechanics and cybernetic physics proposes a way to modeling high-rate processes in condensed media at two scale levels simultaneously with feedbacks. At macroscopic level we use the generalized nonlocal hydrodynamic equations with memory and at intermediate between macro and micro levels we describe dynamics of the space-tame correlations. Self-consistent interrelation between the two levels allows us to include thermodynamic temporal evolution into description of the system out of equilibrium. It was shown that constraints imposed on the system via boundary conditions give rise to new dynamic structures that become momentum and energy carriers. The size spectrum of the structures is discrete as in quantum mechanics. During the system relaxation to equilibrium the spectrum evolves and becomes continuous near equilibrium where the continuum mechanics is valid. In condensed media where internal interaction and inertial forces are strong the nonlocal and memory effects are most pronounced. In experiments on the shock loading of solid materials [7,8] self-organization of new rotational structures at mesoscopic scale level between the atom/dislocation scale level and the macroscopic scale had been found out and it was concluded that the observed patterns of the wave propagation can only be explained via the structure evolution included into the process model.

In the paper first, to facilitate understanding, we briefly outline the main points of the approach used. In the second half we apply the proposed approach to one of the test problems in mechanics in order to demonstrate its ability. The problem on mathematical modeling shear processes in condensed matter out of equilibrium is of interest both for theory and for practical use. Several explicit approximate solutions to the problem in the framework of the proposed approach show that the shear stress and the integral entropy production far from equilibrium decrease compared with Newtonian fluid at the same conditions and the obtained nonlinear velocity profiles become unstable due to the dynamic structure evolution which generates longitudinal pressure gradients near the walls. It means that far from equilibrium due to the self-consistency of the nonlocal model the shear stress changes and the shear flow becomes non-stationary. The obtained results give new opportunity to control the system evolution and to predict final states of the system.

2. New approach to non-equilibrium transport processes

2.1. The problem of closing the transport equations

Transport of mass, momentum and energy follows all real physical processes. For distributed macroscopic systems the mass ρ , momentum $\mathbf{p} = \rho\mathbf{v}$ and internal energy E volume densities are used to describe the transport processes in media of various nature. The densities satisfy the general transport equations

$$\frac{\partial \rho a}{\partial t} + \nabla \cdot \mathbf{J} = I, a = 1, \mathbf{v}, E. \quad (1)$$

Here \mathbf{J}, I are the mass, momentum and energy fluxes and sources respectively. If the fluxes are expressed in terms of the densities and the sources are given, the transport equations govern the macroscopic fields

of distributed mass, momentum and energy during the physical process. However, the problem is complete only in two limiting cases: for small velocity gradients or strain-rates (classical hydrodynamics) and small deformations (theory of elasticity). In both cases the transport equations are the partial differential ones derived under the condition $l \ll |a|/|\text{grad}|a||$. It means that effects of the internal structure (with elements of the typical linear size element l) can be neglected for low-gradients processes. For high-rates and large deformations the problem of closing the transport equations is still exists. Numerous attempts of modeling processes far from equilibrium based on empirical differential equations failed. Such models did not have predictive ability in a wide range of conditions because they did not meet the changing system responds to external loading.

2.2. Thermodynamic relationships in non-equilibrium statistical mechanics

From the point of view of the non-equilibrium statistical mechanics the general transport equations are not entirely localized far from equilibrium [1,2,3]. D.N. Zubarev [3] derived generalized integral thermodynamic relationships valid out of equilibrium from the first principles by the method of non-equilibrium statistical operator. The general relationships between the conjugate thermodynamic fluxes \mathbf{J} and forces \mathbf{G} (gradients of macroscopic variables) including nonlocal and memory effects have an integral form

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^t dt' \int_V d\mathbf{r}' \mathbf{R}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{G}(\mathbf{r}', t'). \quad (2)$$

The weight function \mathbf{R} (the tensor rank of the function \mathbf{R} is double the rank of the tensor \mathbf{G}) in the integral relationships (2) is a space-time correlation function depending on the history of statistical distribution function all over the system volume. It means that the temporal system evolution out of equilibrium is included in the description of each thermodynamic state at any spatial point. In the general case the non-equilibrium correlation function is unknown nonlinear functional of macroscopic gradients \mathbf{G} .

In accordance with Bogoliubov's hypothesis the initial space-time correlations are decaying during the system relaxation to equilibrium. The relationships (2) with nonlocal and memory effects neglected become the known linear thermodynamic relationships of irreversible transport

$$\mathbf{J}(\mathbf{r}, t) = k_o(\mathbf{r}, t) \mathbf{G}(\mathbf{r}, t), \quad k_o(\mathbf{r}, t) = \int_{-\infty}^t dt' \int_V d\mathbf{r}' \mathbf{R}(\mathbf{r}, \mathbf{r}', t, t') \quad (3)$$

In the general case the transport coefficients $k_o(\mathbf{r}, t)$ in (2) depend on the system volume, geometry and boundary conditions. Near the local equilibrium the coefficients $k_o(\mathbf{r}, t)$ become constant representing only the medium properties in accordance with linear thermodynamics of irreversible transport processes [9]. The equations describing mass, momentum and energy transport are differential equations of continuum mechanics. Out of equilibrium the equations (1) with fluxes in the integral form (2) are nonlocal and with memory effects.

It was shown [3] that unlike linear thermodynamics of irreversible processes the local entropy production $\sigma(\mathbf{r}, t) = \mathbf{J} \cdot \mathbf{G}$ (here we mean the summation over fluxes and forces) can change its sign during non-equilibrium processes. If only nonlocal effects are taken into account, the integral entropy production at any time is non-negative $\int_{-\infty}^t dt' \int d\mathbf{r} \sigma(\mathbf{r}, t') \geq 0$. Accounting both nonlocal and memory effects provides non-negative value of only total entropy generation after non-equilibrium process is fully completed $S(+\infty) - S(-\infty) = \int_{-\infty}^{+\infty} dt \int d\mathbf{r} \sigma(\mathbf{r}, t) \geq 0$.

2.3. Dynamic self-organization during non-equilibrium transport

In the general case the space-time correlations can not be separated. Since spatial and temporal scales of non-equilibrium process are different it becomes possible to consider either nonlocal effects or memory. In synergetics the separation of the process scales is the necessary condition for self-organization. In transient processes nonlocal and memory effects play different roles at initial and final

stages of the process [6]. For quasi-stationary high-rate processes the relationships (2) include only nonlocal effects. For simplicity and keeping in mind application of the approach to pure shear problem in the next section, further we consider only 1-dimensional case for relationships (2) in the form

$$J(y) = \eta \int_a^b dy' \Psi(y, y') G(y'), \quad J(y) \rightarrow \eta \int_a^b dy' \delta(|y' - y|) G(y') = \eta G(y) \quad (4)$$

In the limiting case close to local equilibrium the nonlocal effects disappear and the relationships between $J(y)$ and $G(y)$ tends to the linear thermodynamic relationships of irreversible transport processes. Expansion of the function $G(y)$ in a Taylor series near the point $y' = y$ and its substitution into Eq (4) leads to an infinite order differential operator

$$\int_a^b dy' \Psi(y, y') G(y') = k_0(y) G(y) + k_1(y) \frac{\partial G}{\partial y}(y) + \frac{1}{2} k_2(y) \frac{\partial^2 G}{\partial y^2}(y) + \dots \quad (5)$$

The coefficients in the expansion (5) can be called moments of the spatial correlation function

$$k_n(y) = \int_a^b \Psi(y, y') (y - y')^n dy' \quad (6)$$

The infinite set of the moments is equivalent to the correlation function but finite is not. The 0-order moment $k_0(y)$ defines the generalized transport coefficient $\eta k_0(y)$. The 1-order moment $k_1(y) = \gamma(y)$ (in 3-D it is a vector). Near the local equilibrium with nonlocal effects neglected $\Psi(y, y') = \delta(|y' - y|)$ the first order moment $\gamma(y) = 0$ disappears. It should be noticed that in 3D case the first order moment is a vector. It means that out of equilibrium new direction and new typical length generated by non-equilibrium correlations give rise to the medium polarization. The 2-order moment defines the dispersion ε^2 of the space correlation distribution which due to due to γ becomes eccentric $\gamma(y)$

$$\int_a^b \Psi(y, y') (y - y')^2 dy' = \int_a^b \Psi(y, y') (y'^2 - y^2) dy' - 2y\gamma(y) = \varepsilon^2(y) - 2y\gamma(y)$$

The higher order moments have no physical meaning but should not be neglected out of equilibrium. In the general case the moments depend on the system size and its geometry. The finite order differential operator with truncated sums can be used only for rather small gradients i.e. near local equilibrium. Close to local equilibrium the transport equations (1) are differential ones. In continuum mechanics the correlations disappear and the transport mechanisms become independent on boundary conditions and external actions. That's why the equations of continuous mechanics cannot describe transient processes.

Parameters γ and ε have the dimensions of length. The medium element of the typical size ε moving as eccentric cluster in inhomogeneous velocity and stress fields should rotate as a whole. Such vortices can be considered as the finite size dynamic structure of the bounded system. So, out of equilibrium i.e. at high-rates and high gradients the spatial nonlocal correlations generate the vortex turbulent structures. Such self-organization of new dynamic structures occurs only due to non-equilibrium spatial correlations and shear processes near boundaries. In condensed matter the dynamic structures in irreversible process can result in a new spatial internal structure frozen into material of the system.

2.4. Modeling the correlation functions

Since the explicit form of the correlation function is unknown, the only possible way to use nonlocal transport equations out of equilibrium is to model the correlation function. The required model should be δ -type to provide the transition to classical hydrodynamics near local equilibrium. Then the model should include the main physical properties of the correlation distribution that are given by the first its moments. However, the model thermodynamic relationships should remain integral out of equilibrium. The simplest δ -type form of the distribution is gaussian with the first three moments included according to their physical meaning.

The 3-parameters approximation for the correlation function in quasi-stationary processes takes a form [6]

$$\Psi_a(y, y'; \gamma_a, \varepsilon_a) = \frac{1}{\varepsilon_a} \exp\left\{-\frac{\pi(y'-y+\gamma_a)^2}{\varepsilon_a^2}\right\} \xrightarrow{\gamma_a \rightarrow 0, \varepsilon_a \rightarrow 0} \delta(|y' - y|) \quad (7)$$

Here the sequence of the transition to the limit is fixed to embrace correlations with boundaries. The approximate correlation function is scalar, not tensor, the flux of each value a is characterized by its own parameters γ_a and ε_a . Further for simplicity index a will be omitted.

In papers [6,8,10,11] the model correlation function in the form (7) is used for several mechanical problems. Its dependence on the first moments made it possible to reveal some special effects accompanying transport processes far from equilibrium.

However, the problem of closing the transport equations is still remained unsolved. The model parameters γ and ε remained unknown functionals of gradients G as well as the correlation function itself. It should be noted an important circumstance that the transport equations (1) with the fluxes (4) taking into account the nonlocal correlations are integral-differential. In the general case boundary conditions imposed on the system to solve boundary problems for the 2-order differential hydrodynamic equations are not satisfied for nonlocal equations. Then one can try to satisfy the boundary conditions imposed on the system due to the parameters of the space correlation function $\Psi(y, y'; \gamma, \varepsilon)$ in the form (7). For stationary processes the transport equations (1) on the boundary conditions at $y = b, c$ can result in a set of nonlinear equations with respect to the parameters γ and ε for all values a

$$(\nabla \cdot J_a(y; \gamma_a, \varepsilon_a) - I_a(y)) \Big|_{y=b, c} = 0, \quad a = 1, v, E \quad (8)$$

In the general case the structure parameters are implicitly expressed through macroscopic fields all over the system including boundaries via conditions (8). However, boundary conditions (8) can determine only mean values of the parameters or if their dependence on y is given by the system geometry. Since finite values of the model parameters can represent linear sizes of the system dynamic structure, equations (8) determine dynamic self-organization in the system [6,8,10]. Like in quantum mechanics, the bounded system out of equilibrium can have a discrete spectrum of the structure sizes or continuous spectrum near equilibrium where differential equations of continuous mechanics (not related to the boundary conditions) are valid. So, external actions across borders keeping the system far from thermodynamic equilibrium can generate various turbulent structures.

We can conclude that the self-organization appears to be the necessary component of the transport processes modeling far from equilibrium.

2.5. Internal control and the structure evolution

However, in the general case the number of the boundary conditions is less than the number of the structure parameters. Therefore, the set (8) determines only interrelations between the structure parameters. Macroscopic boundary conditions are not sufficient to find all the structure parameters. A part of them evolves, the rest part via interrelations evolves too and the macroscopic system also evolves tending to reach a more stable state under the imposed conditions. In accordance with the Gibbs-Jaynes principle of the maximum entropy [12,13] the entropy of any physical system tends to grow until it reaches the maximum possible value under constraints imposed. The speed-gradient principle [4,14] developed in the control theory of adaptive systems defines the law by which it will evolve. In paper [15] the entropy generated in the system during the relaxation process under the imposed constraints takes a form

$$\Delta S(t) = \sum_a \int_0^t dt \int_b^c dy J_a(y; \gamma_a, \varepsilon_a) \frac{d}{dy} a(y) + \sum_a \lambda_{ab} \left[\left(\frac{d}{dy} J_a(y; \gamma_a, \varepsilon_a) - I_a(y) \right) \Big|_{y=b} \right] +$$

$$+ \sum_a \lambda_{ac} \left[\left(\frac{d}{dy} J_a(y; \gamma_a, \varepsilon_a) - I_a(y) \right) \Big|_{y=c} \right], a = 1, v, E \quad (9)$$

The coefficients $\lambda_{ab}, \lambda_{ac}$ are Lagrange multipliers. Maximum value of the functional ΔS is chosen for a goal functional of the system evolution. According to the SG-principle among all process scenarios, only one is realized, which ensures the quickest achievement of the goal due to the control parameters evolution. The sets of the structure parameters rates $\langle d\gamma_a(t)/dt, d\varepsilon_a(t)/dt \rangle$ are chosen as control parameters. First, we take the time derivative of $\Delta S(t)$ to define its maximum

$$\begin{aligned} \frac{d}{dt} \Delta S(t) = & \sum_a \int_b^c dy J_a(y; \gamma_a, \varepsilon_a) \frac{d}{dy} a(y) + \sum_a \lambda_{ab} \frac{d}{dt} \left[\left(\frac{d}{dy} J_a(y; \gamma_a, \varepsilon_a) - I_a(y) \right) \Big|_{y=b} \right] + \\ & + \sum_a \lambda_{ac} \frac{d}{dt} \left[\left(\frac{d}{dy} J_a(y; \gamma_a, \varepsilon_a) - I_a(y) \right) \Big|_{y=c} \right], a = 1, v, E \end{aligned} \quad (10)$$

The expression (10) without the constraints imposed by the boundary conditions defines the integral entropy production as the sum of the products of thermodynamic forces and fluxes. Since the entropy generation reaches its maximum, the integral entropy production as a rate of the entropy generation becomes 0. Under the constraints it is not so. In paper [15] we have shown that the final entropy generation of the whole system under constraints is always lower than during free relaxation and the integral entropy production reaches a nonzero minimum in steady state [16].

For quasi-stationary processes $d\Delta S/dt$ depends on time only via the set of the parameters $\langle \gamma_a(t), \varepsilon_a(t) \rangle$ and does not depend on their rates $\langle d\gamma_a(t)/dt, d\varepsilon_a(t)/dt \rangle$. In order to get the dependence it is necessary to differentiate the integral entropy production by time to define its minimum. Easy to see that for quasi-stationary processes the SG-algorithm coincides to conventional gradient descent algorithm with the goal function $d\Delta S/dt$ and the control parameters $\langle \gamma_a(t), \varepsilon_a(t) \rangle$. Let $\zeta(t)$ be one of the set of the parameters $\langle \gamma_a(t), \varepsilon_a(t) \rangle$. Then we get

$$\nabla_{d\zeta/dt} \left(\frac{d^2}{dt^2} \Delta S \right) = \nabla_{d\zeta/dt} \left[\nabla_{\zeta} \left(\frac{d}{dt} \Delta S \right) \frac{d\zeta}{dt} \right] = \nabla_{\zeta} \left(\frac{d}{dt} \Delta S \right). \quad (11)$$

The speed-gradient algorithm in a finite form [4,15] defines the system evolution by a set of the 1st order differential equations with respect to the set of the structure parameters $\langle \gamma_a(t), \varepsilon_a(t) \rangle$

$$\frac{d\varepsilon_a}{dt} = -g_{a\varepsilon} \frac{\partial}{\partial \varepsilon_a} \left(\frac{d}{dt} \Delta S(t; \langle \gamma_a(t), \varepsilon_a(t) \rangle) \right), \quad \frac{d\gamma_a}{dt} = -g_{a\gamma} \frac{\partial}{\partial \gamma_a} \left(\frac{d}{dt} \Delta S(t; \langle \gamma_a(t), \varepsilon_a(t) \rangle) \right). \quad (12)$$

The algorithm (11) can be interpreted as follows. Over multidimensional space of the control parameters $\langle \gamma_a(t), \varepsilon_a(t) \rangle$ hyper-surface $\frac{d}{dt} \Delta S(t; \langle \gamma_a(t), \varepsilon_a(t) \rangle)$ is constructed. Paths of the system evolution are descending along the surface gradients. Finite states of the system depend on the initial point in the space of the control parameters corresponding to the initial system structure. If the initial point is on a part of the surface with 0 gradients, the system state is stable. If it is on the slope part, the system will evolve until it reaches a stable state. During the system evolution far from equilibrium feedbacks between the structure evolution via $\langle \gamma_a(t), \varepsilon_a(t) \rangle$ and the macroscopic system evolution via $\Delta S(t; \langle \gamma_a(t), \varepsilon_a(t) \rangle)$ arise. Due to the feedbacks the hyper-surface changes its form and the evolution paths can change too. As a result meta-stable states may occur in which the system can change direction of its evolution at very low external action. System in this state is easy to control in order to get its state with the desired structure.

3. Pure shear processes in nonlocal hydrodynamics

3.1. Formulation of the problem

As an example, consider the use of models of nonlocal hydrodynamics for high-rate shear processes in condensed matter. The problem of pure shear in hydrodynamics had been formulated by Couette [17,18]. Two infinite parallel plates at a distance $2h$ from each other move at a constant velocity U in opposite directions. For the steady flow of Newtonian fluid the shear stress between the plates is constant $S_{xy} = \mu du/dy = \text{const}$ (x, y are coordinates in the longitudinal and transverse directions relative to the plates, μ is shear viscosity and $u(y)$ is longitudinal mass velocity). Under the sticking conditions $u(\pm h) = \pm U$ linear velocity profile $u(y) = (U/h)y$ is established. In dimensionless form one gets

$$S = \frac{du}{dy} = 1, \quad u(\pm 1) = \pm 1, \quad u(y) = y \quad (13)$$

High-rate shear in condensed medium can not be described by Newtonian fluid model. High-rate interaction of the medium with rigid boundaries results in a complex of non-equilibrium effects that can make the velocity profile nonlinear and change shear stress. Out of equilibrium viscous properties of the medium are associated not so much with the properties of the medium itself, as with the properties of the entire system, its geometry, sizes, distance to the boundaries and interaction with the walls. Such behavior of the viscosity was observed in fluids at high-rates [19]. Just the same effects had been found for flows in nanotubes by simulation of the correlation functions in the framework of Zubarev's nonlocal hydrodynamics [20]. The empiric coefficient μ defines only properties of the fluid under close-to-equilibrium conditions. Therefore in order to analyze the shear flow under non-equilibrium conditions we apply for the stress component S the nonlocal model (4) with the correlation function in the form (7). The correlation function (7) is modified ($\gamma = \beta y$ [6]) to account for the given symmetry properties of the flow. Dimensionless model expression for the shear stress component takes a form

$$S(y) = \varepsilon \int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left\{-\frac{\pi}{\varepsilon^2}(y' - y(1 - \beta))^2\right\} \frac{\partial u}{\partial y'} \xrightarrow{\beta, \varepsilon \rightarrow 0} \varepsilon \int_{-1}^1 dy' \delta\{|y' - y|\} \frac{\partial u}{\partial y'} = \varepsilon \frac{\partial u}{\partial y} \quad (14)$$

The model (14) generalizes Newtonian model to the case of stationary non-equilibrium processes. The dimensionless parameters ε, β describe nonlocal and boundary effects omitted in the Newtonian model. Here we consider the viscosity out of equilibrium conditions $\mu = \mu_0 \varepsilon$ depending on the correlation length.

3.2. Newtonian model with an effective viscosity as zero approximation

For high-rate flows and the structured medium values of the parameters ε, β are finite. In the zero approximation instead of (1) we get Newtonian model with an effective viscosity

$$S(y) = \varepsilon \int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left\{-\frac{\pi}{\varepsilon^2}(y' - y(1 - \beta))^2\right\} \frac{\partial u}{\partial y'} = \varepsilon k_0(y; \varepsilon, \beta) \frac{\partial u}{\partial y} \quad (15)$$

The effective viscosity $\mu_0 \varepsilon k_0$ is not constant. Through the zero moment of the correlation function it is associated with the integral properties of the system including boundary conditions

$$\begin{aligned} k_0(y; \varepsilon, \beta) &= \int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left\{-\frac{\pi}{\varepsilon^2}(y' - y(1 - \beta))^2\right\} = \\ &= \frac{1}{2} \left[\operatorname{erf}\left\{\frac{\sqrt{\pi}}{\varepsilon}(1 - y(1 - \beta))\right\} + \operatorname{erf}\left\{\frac{\sqrt{\pi}}{\varepsilon}(1 + y(1 - \beta))\right\} \right] \xrightarrow{\varepsilon \rightarrow 0} 1 \end{aligned}$$

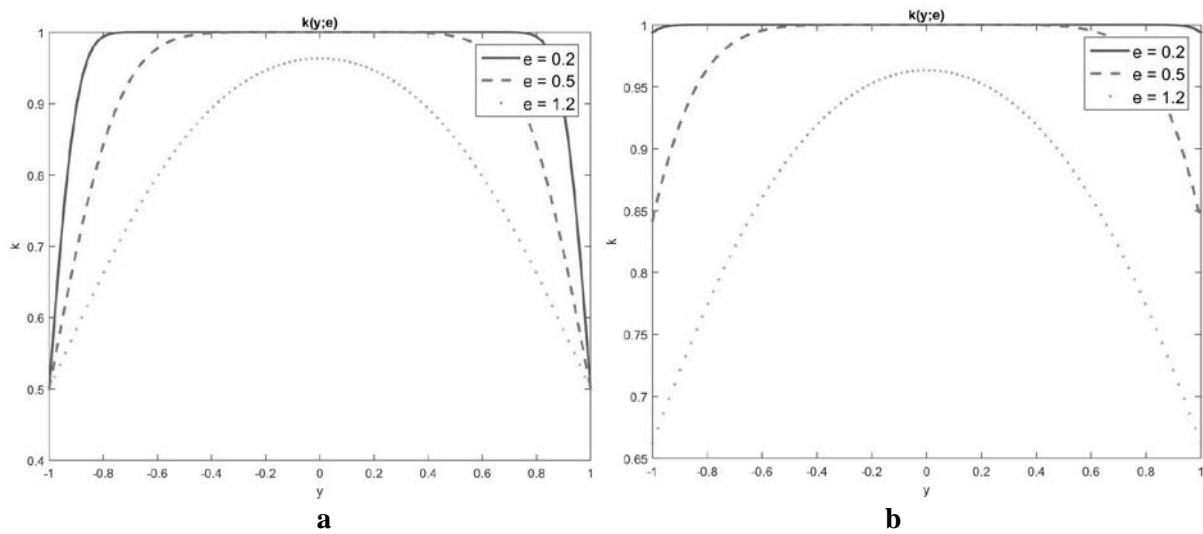


Figure 1. a) The dependence $k_0(y; \varepsilon, \beta = 0)$ for $\varepsilon = 0.2, 0.5, 1.2$;
b) The dependence $k_0(y; \varepsilon, \beta = 0.2)$ for $\varepsilon = 0.2, 0.5, 1.2$

Fig.1 shows that the effective viscosity reduces near boundaries whereas in the central part it is almost constant:

$$k_0(y; \varepsilon) \approx k_0(0; \varepsilon) = \operatorname{erf} \frac{\sqrt{\pi}}{\varepsilon}, \quad k_0(\pm 1; \varepsilon, \beta) = \frac{1}{2} \left[\operatorname{erf} \left\{ \frac{\sqrt{\pi}}{\varepsilon} \beta \right\} + \operatorname{erf} \left\{ \frac{\sqrt{\pi}}{\varepsilon} (2 - \beta) \right\} \right] \leq \operatorname{erf} \left\{ \frac{\sqrt{\pi}}{\varepsilon} \right\}$$

It is interesting to notice that the effect of the viscosity reduction near boundaries had been found in the flows of some dispersed media such as blood, for example [21]. However, Newtonian model even with an effective viscosity cannot be used far from equilibrium.

3.3. Pure shear with nonlocal effects

In the general case for pure shear we have $S = \varepsilon \chi(\varepsilon, \beta)$ that results in an integral-differential equation with respect to the $u(y)$

$$\int_{-1}^1 \frac{dy'}{\varepsilon} \exp \left\{ -\frac{\pi}{\varepsilon^2} (y' - y(1 - \beta))^2 \right\} \frac{\partial u}{\partial y'} = \chi(\varepsilon, \beta) \quad (16)$$

Finding the velocity profile from the equation (16) is incorrect problem. To solve such problems regularization methods should be used. First rewrite (16) to gain an integral equation with respect to the velocity $u(y)$. Integrating (16) in parts on the sticking boundary conditions and taking into account that $\partial/\partial y' = -(1 - \beta)^{-1} \partial/\partial y$, we obtain an integral equation

$$\frac{1}{1 - \beta} H(y; \varepsilon, \beta) + \frac{1}{1 - \beta} \int_{-1}^1 \frac{dy'}{\varepsilon} \exp \left\{ -\frac{\pi}{\varepsilon^2} (y' - y(1 - \beta))^2 \right\} u(y') = \chi y, \quad (17)$$

where $H(y; \varepsilon, \beta) = \frac{1}{2} \left[\operatorname{erf} \left\{ \frac{\sqrt{\pi}}{\varepsilon} (1 + y(1 - \beta)) \right\} - \operatorname{erf} \left\{ \frac{\sqrt{\pi}}{\varepsilon} (1 - y(1 - \beta)) \right\} \right]$.

The equation (17) includes three unknown parameters ε, β, χ which are all interconnected through the nonlocal correlation. By adding $u(y)$ to both parts of (17) and using the sticking boundary conditions we can get a set of nonlinear operator equations with respect $u(y)$ and the parameters ε, β, χ

$$u(y) = u(y) + \chi y - \frac{1}{1 - \beta} H(y; \varepsilon, \beta) - \frac{1}{1 - \beta} \int_{-1}^1 \frac{dy'}{\varepsilon} \exp \left\{ -\frac{\pi}{\varepsilon^2} (y' - y(1 - \beta))^2 \right\} u(y'), \quad (18)$$

$$1 = u(1) + \chi - \frac{1}{1-\beta} H(1; \varepsilon, \beta) - \frac{1}{1-\beta} \int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left\{-\frac{\pi}{\varepsilon^2} (y' - (1-\beta))^2\right\} u(y'). \quad (19)$$

Due to oddness of the function $u(y)$ the second condition at $y = -1$ is identical to (19). In order to determine all the parameters ε, β, χ we need two relationships additionally. If the value $\chi(\varepsilon, \beta)$ considers being constant for pure shear we can use the equation (16) at $y = 0$

$$\int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left\{-\frac{\pi}{\varepsilon^2} (y')^2\right\} \frac{\partial u}{\partial y'} = \chi(\varepsilon). \quad (20)$$

An approximate solution to the set of nonlinear equations (18)-(20) can be obtained by iteration method developed in the theory of nonlinear operator systems [22]. The iteration scheme for the set (18)-(20) is chosen as follows

$$u_i(y) = F_\varepsilon[u_{i-1}(y), \beta_i, \chi_i], \quad \Phi_{1\varepsilon}[u_{i-1}(y), \beta_i, \chi_i] = 0, \quad \Phi_{2\varepsilon}[u_{i-1}(y), \beta_i, \chi_i] = 0. \quad (21)$$

In the limiting case $\varepsilon \rightarrow 0$ the nonlocal effects are neglected and the equations (18)-(20) results in the linear velocity profile $u(y) = y$ which is suitable near local equilibrium. For the set (21) the nonlocal parameter ε is considered external. Later we use an algorithm developed in the control theory of adaptive systems for its determination. Let the solution $u_0(y) = y$ is chosen as zero approximation. Substituting it into the right side of the equation (18) and into relationships (19)-(20) we can get a solution in the first approximation

$$u_1(y) = y + \chi y - \frac{1}{1-\beta} H(y; \varepsilon, \beta) - \frac{1}{1-\beta} \int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left\{-\frac{\pi}{\varepsilon^2} (y' - y(1-\beta))^2\right\} y', \quad (22)$$

$$1 = 1 + \chi - \frac{1}{1-\beta} H(1; \varepsilon, \beta) - \frac{1}{1-\beta} \int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left\{-\frac{\pi}{\varepsilon^2} (y' - (1-\beta))^2\right\} y', \quad (23)$$

$$\chi(\varepsilon) = \operatorname{erf}\left\{\frac{\sqrt{\pi}}{\varepsilon}\right\} \quad (24)$$

According to (24) the velocity gradient in the center of the flow decreases with increasing the nonlocal effects

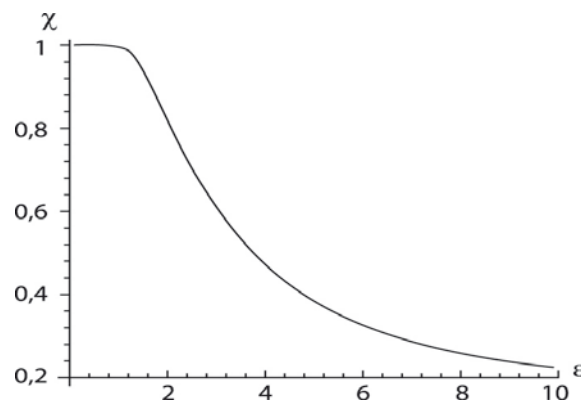


Figure 2. Dependence of the normalized shear stress $\chi(\varepsilon)$ on the non-local parameter ε .

Roots of the transcendent equation (23) with respect to the parameter β define piecewise continuous spectrum of admissible values β

$$\Phi_1(\beta; \varepsilon) = 0, \quad \Phi_1(\beta; \varepsilon) = \chi(\varepsilon)(1-\beta) - H(1; \varepsilon, \beta) - \int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left\{-\frac{\pi}{\varepsilon^2} (y' - (1-\beta))^2\right\} y' \quad (25)$$

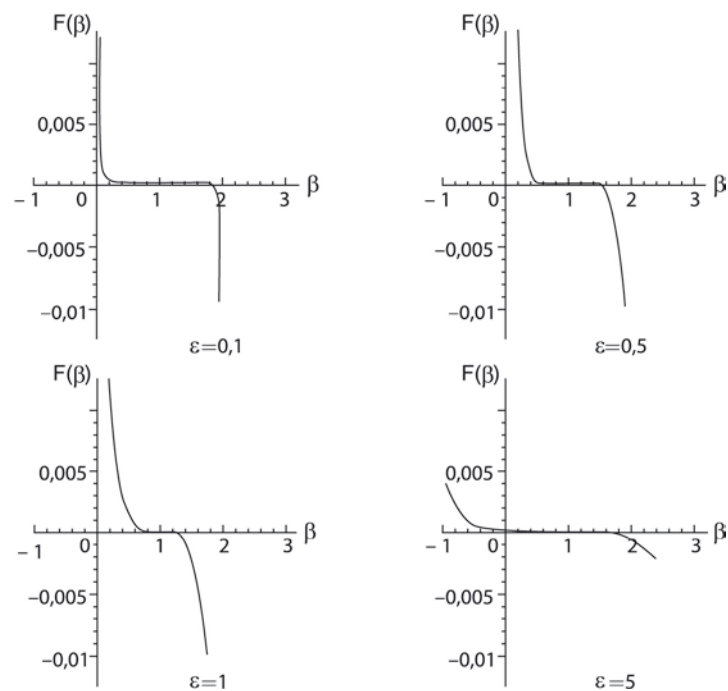


Figure 3. Behavior of the function $\Phi_1(\beta; \varepsilon)$ at various values of ε .

In the regions of continuous values β continuum mechanics is valid. With increasing the non-local parameter ε the region is shrinking to a central point $\beta = 1$ where $u(y, \beta = 1) = 0$, then it is widening again out of the system boundaries and the approximation (22)-(24) loses its physical meaning. For rather small ε near the boundaries there appear layers where continuum mechanics becomes invalid whereas in the center of the flow it still gives linear velocity profiles. However, the velocity profiles in the first approximation and the linear profile $u(y) = y$ turned out to be too close since the sticking conditions are satisfied. As the nonlocal parameter ε grows the value $\chi(\varepsilon)$ decreases and the velocity profiles become linear $u(y) = \chi y$ which do not satisfy the sticking conditions.

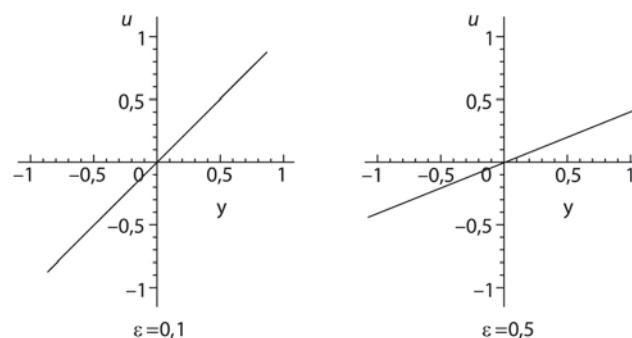


Figure 4. Approximate velocity profiles at various parameters ε .

Inertial effects in condensed matter lead to a lag of the medium behind the plates. Due to the difference between the medium on the boundary and the wall itself a torque occurs inside the near-boundary layers where linear Newtonian model becomes invalid. As the slips on the boundaries increase with the nonlocality parameter ε , the rotation moments also increase as well as the lag of the medium behind the

plates. Since the nonlocal correlations embrace all medium between the plates the external torque tries to rotate the medium as a whole but the internal medium rotation arising due to the inertial effects in the opposite direction prevents this. In balance the internal and external torques cancel each other out, the medium remain immobile. In unstable state separate parts of the medium can rotate forming complicated dynamic structures [23-29].

A scheme of the movements between the plates at various values of the nonlocality parameter ε is presented in Fig. 5

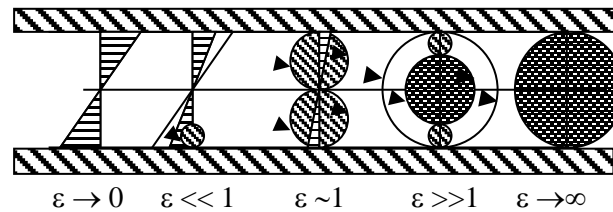


Figure 5. Scheme of the movements between the plates at various values of the nonlocality parameter ε .

Choosing the solution $u_0(y) = \chi y$ with the slips on the walls as zero approximation we get discrete spectrum of the admissible values β . In Fig. 6 the roots of the equation

$$\chi(\varepsilon) \left[(1 - \beta) - H(1; \varepsilon, \beta) - \int_{-1}^1 \frac{dy'}{\varepsilon} \exp \left\{ -\frac{\pi}{\varepsilon^2} (y' - (1 - \beta))^2 \right\} y' \right] = (1 - \beta)(1 - \chi) \quad (26)$$

are presented. Unlike (25) the slip on the walls makes the right side of (26) non-zero.

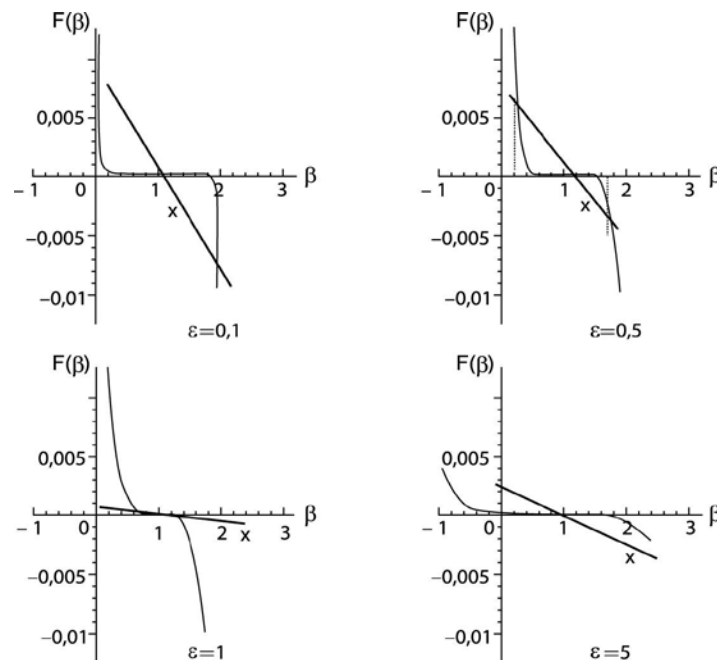


Figure 6. The admissible values β at various parameters ε .

Here we can see that two roots exist at rather small values of nonlocality ε which allow us to satisfy the sticking boundary conditions. At large nonlocality only one root corresponding to the trivial solution

$u(y, \beta = 1) = 0$ exists in the balance between the torques. Both roots β_1, β_2 lead to nonlinear velocity profiles meeting the sticking conditions on the boundaries (Fig. 7). The root $\beta_1 < 1$ corresponds to the velocity profile similar to non-stationary one in the flow with acceleration (left). Nonlinear velocity profile with the root $\beta_2 > 1$ looks like in braking flow (right). In both cases the inertia of condensed matter results in non-equilibrium interaction with rigid boundaries.

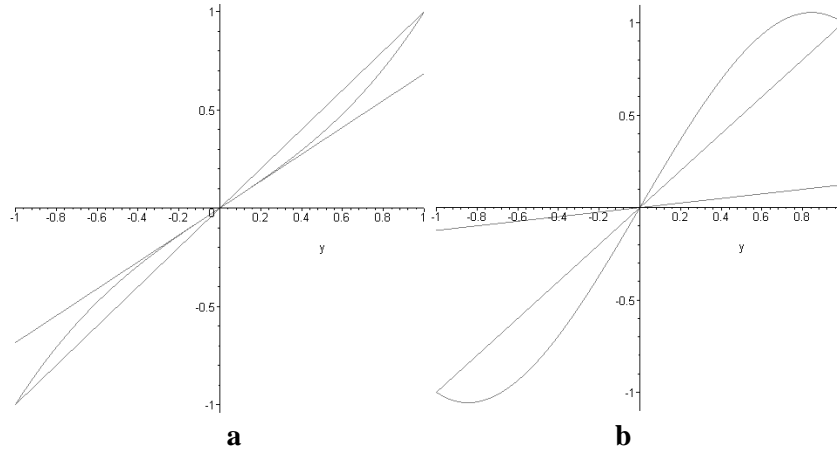


Figure 7. a) Velocity profiles for β_1 b) Velocity profiles for β_2

In hydrodynamics it is known that the presence of mixing pulsations in the liquid leads to equalization of velocities in the middle part of the pressureless Couette flow. This fact corresponds to the velocity gradient reduction in the center of the turbulent flow $\chi(\varepsilon) \leq 1$ for finite values of the nonlocal parameter ε . It is interesting to notice that in high-rate shear flows local pressure gradients occur near boundaries and generate local accelerations which make the flow unstable [30,23,27,28].

3.4. Stability of high-rate pure shear

In order to consider the stability of the non-equilibrium shear flow we use SG-principle in accordance with the algorithm presented in section 2.6 of the paper. According to the principle of maximum entropy the flow field evolves until the value of the full entropy generation reaches maximum in the most stable state on the given conditions. First consider the stability of the solution $u(y) = \chi(\varepsilon)y$ with slips on the boundaries. In the general case the solution is considered quasi-stationary because it can depend on time only via the nonlocal parameter $\varepsilon(t)$. The normalized shear stress is $\varepsilon\chi(\varepsilon)$ because out of equilibrium the shear viscosity $\mu \sim \varepsilon$ grows with the nonlocal correlations. The full entropy generation is $\Delta S(\varepsilon) = \int_{-\infty}^t dt \int_{-1}^1 dy \varepsilon \chi^2(\varepsilon) y$. The only control parameter is the nonlocality parameter $\varepsilon(t)$ which is responsible for the dynamic structure evolution. The rate of the entropy generation is the integral entropy production $\Omega(\varepsilon) \equiv \frac{d\Delta S(\varepsilon)}{dt} = \int_{-1}^1 dy \varepsilon \chi^2(\varepsilon) y = 2\varepsilon \chi^2(\varepsilon)$. The SG algorithm defines the rate of the structure evolution $\frac{d\varepsilon}{dt} = -g \frac{\partial}{\partial \varepsilon} (\Omega(\varepsilon))$. According to SG-algorithm the evolution path goes down the curve $\Omega(\varepsilon)$. The function $\Omega(\varepsilon)$ is a non-monotone because $\Omega(\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} 0$ (limit of ideal fluid) and $\Omega(\varepsilon) \xrightarrow{\varepsilon \rightarrow \infty} 0$ (limit of rigid body). The function has maximum at $\varepsilon = \varepsilon^*$. It means that depending on the initial value $\varepsilon(t = 0)$ two directions of the structure evolution are possible.

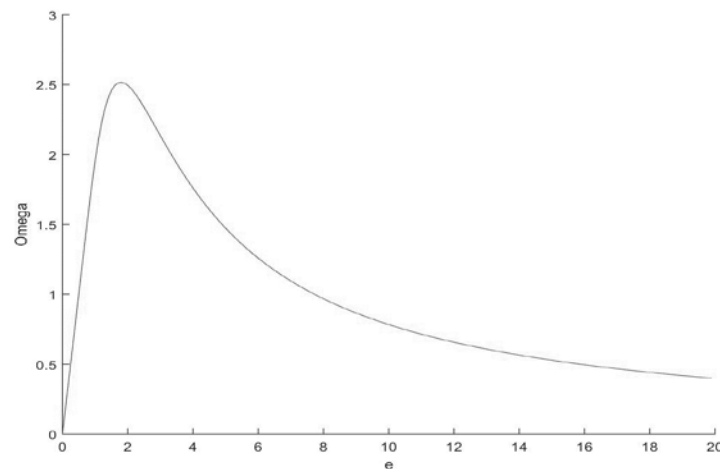


Figure 8. Dependence of the integral entropy production $\Omega(\varepsilon)$ on the nonlocal parameter ε .

Taking the time derivative of the flow velocity $\partial u/\partial t = y(\partial\chi/\partial\varepsilon)(\partial\varepsilon/\partial t)$ one can estimate the influence of the system structure evolution. In the flow with initial dynamic structure $\varepsilon(t=0) < \varepsilon^*$ the space correlations weaken $\partial\varepsilon/\partial t < 0$. The structure temporal evolution induces local accelerations along the stream $\partial u/\partial t > 0$ since $\partial\chi/\partial\varepsilon \leq 0$ is always non-positive (See Fig.4). If $\varepsilon(t=0) > \varepsilon^*$ the nonlocal correlations grow $\partial\varepsilon/\partial t > 0$ forming large vortices which slow down the movement $\partial u/\partial t < 0$. Eventually the correlations embrace the plates and the flow stops moving. Any non-equilibrium flow with the velocity profile $u(y) = \chi y$ ($\chi(\varepsilon) < 1$) is unstable. In both limiting cases due to the structure evolution the flow tends to the steady equilibrium state with zero velocity. Without the constraints imposed on the flow by the sticking boundary conditions the stable non-equilibrium state is not reached because there is no interaction between the medium and the plates. The flow with the velocity profile $u(y) = \chi(\varepsilon^*)y$ is meta-stable. Any velocity fluctuation can change the evolution direction.

3.5. Non-stationary formulation

So, in the general case out of equilibrium it is necessary to analyze non-stationary formulation of the problem.

$$\frac{h}{CT} \frac{\partial u}{\partial t} = \frac{\partial}{\partial y} \left(\varepsilon \int_{-1}^1 \frac{dy'}{\varepsilon} \exp\left(-\frac{\pi(y'-y(1-\beta))^2}{\varepsilon^2}\right) \frac{\partial u}{\partial y'} \right) \quad (27)$$

Here C is the sound velocity, T is the steady state establishment time. At $T \rightarrow \infty$ we come to the formulation (3). The dependence of the nonlocal parameter ε on the plates velocity U is different for each system and can be determined experimentally.

Unlike the quasi-stationary case the non-stationary formulation should take into account feedbacks between the velocity profiles and the structure evolution. Then during the structure evolution the integral entropy production should change too, changing the flow velocity. The process can be traced only numerically. Calculation in paper [31] based on several nonlocal models show that without feedbacks the calculations may lead to the solutions that have no physical meaning but with their accounting much more stable states can be reached.

4. Conclusion

In order to construct closed mathematical model of a system out of thermodynamic equilibrium new theoretical approach based on non-equilibrium statistical mechanics and methods of cybernetical

physics had been proposed. In the framework of the approach self-organization of dynamic structures and the structure temporal evolution with feedbacks between two scale levels can be considered.

The developed mathematical model with nonlocal correlations included is applied to describe high-rate shear flow on a wide range of conditions. With increasing the flow velocity the laminar-turbulent transition occurs and the velocity profile becomes nonlinear. Near the rigid boundaries rotational structures are generated as a result of non-equilibrium interaction between the liquid and the walls. Such regions are well known in solid mechanics as kink bands or misorientation bands. The turbulent mode of the shear flow due to the structure evolution is unstable in the first approximation. In this approximation the feedbacks between the velocity field and evolving internal structure of the flow are omitted. The feedbacks accounting should decrease gradients and stabilize the flow. However, it is too cumbersome to show explicitly. Numerical calculations show that feedbacks make solutions much more stable though also face difficulties and need further development of new mathematical methods. That is why as long as physicists would use equilibrium rigid models of high-rate processes without involving of the internal structure evolution they will never close the gap between the theory and the modern practical needs.

The proposed approach opens new control capabilities of transient processes and can have an important meaning for the development of new thin technologies, biomechanics, medicine and prediction of multi-scale catastrophic phenomena.

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