Possibilities of Simulation of the Socio-Political Conflicts Based on the Mathematical Technique of the Langmuir Monolayers Theory

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Keywords: Monolayer, Mathematical Simulation, Socio-Political Processes, Socio-Political Conflicts.

Abstract: The possibility of creating the model of social and political processes (in particular, that of conflicts) with use of the chemical theory of monolayers is studied. The main theoretical approaches to simulation of the social processes are analyzed. A formalized dynamic parameters of protest pro-cesses in the crowd are defined. The mathematical model based on the chemical theory of mono-molecular layers and the coupling field parameter (h) are proposed. In addition, the basic equations are derived, interpreted and applied to social processes. The main effects in the studied pro-cesses are described.

1 INTRODUCTION

The question on forecasting the social and political conflicts, including that by means of mathematical simulation, is of the most actuality, especially in the conditions of increasing geopolitical confrontation.

In terms of classical approaches developed earlier, a social conflict is defined in general as a terminal phase in increased confrontation of interests between single individuals, groups of people or in society at whole. This phase is featured by incongruity of separate interests, goals and positions of the interacted subjects. Conflicts can be hidden or explicit, but they are always based on the unwillingness to compromise or even on the complete absence of dialogue between the opposing sides (Dahrendorf, 1965; Gurr and Harff, 1994).

As to mathematical models derived from physical and chemical analogies, they are still relatively rare in sociological researches. Nevertheless, there are a number of works concerning a question on simulation of social and political processes, which a certain success has been achieved in - (Mason, 2013; Traud et al., 2011).

The models presented up to date can be divided into three types:

The 1st type are the conceptual models based on identification and analysis of general historical regularities shaped as cognitive schemes and described the logical links between various factors which affect historical processes. Such models are featured by high degree of generalization, but they are still not mathematical ones, being rather logical and conceptual in their nature.

The 2nd type are the particular mathematical models of simulation type which are focused on the certain historical event or phenomenon. In such models, the main attention is paid to analysis and detailed description of factors and processes that effect the phenomena under research. The models of that type work, as a rule, only if the event under consideration is highly localized and limited by duration. These models are "tied" to a specific historical event and are not applicable for a long period of time.

The 3rd type are the mixed models combining the former two ones. These models simulate a certain class of social processes, without claiming to describe

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Petukhov, A., Morozov, A., Selivantyev, Y., Vorotyntsev, I., Raitman, O. and Morozov, N.
Possibilities of Simulation of the Socio-Political Conflicts Based on the Mathematical Technique of the Langmuir Monolayers Theory.
DOI: 10.5220/0012828500003758

In *Proceedings of the 14th International Conference on Simulation and Modeling Methodologies, Technologies and Applications (SIMULTECH 2024)*, pages 392-398
ISBN: 978-989-758-708-5; ISSN: 2184-2841

in detail the features for each specific historical case (Malkov, 2004).

As a rule, the classical theoretical model of dynamic processes in nonlinear systems (an example of which can be social movements too) operates with multidimensional differential equations, mathematical technique of cellular automata, approaches of theory of catastrophes, and that of the theory of self-organized criticality. Stochastic differential equations by Langevin and Ito-Stratonovich are used too, as well as analysis of chaotic systems with reconstruction of stable states (attractors) by time series (Malkov, 2004; Weber et al., 2015).

A number of studies were devoted to ethnical diversity and its impact on economic, social, cultural development and related processes (Weber et al., 2015). These are cross-cutting studies on mutual influence of ethnic and social problems and the economy. They take into account ethnic and cultural factors and their combined impact on possible and running conflicts.

Forecasting and description of social and political processes uses of variety of methods (Mikhailov and Gorbatikov, 2012).

Since social conflicts have a significant impact on society and processes in it, the development of methods and approaches to describe such phenomena, as well as to predict them, is of great im-portance.

The use of the mathematical techniques of Langmuir Monolayers Theory (LMT) for simulations of social conflicts and their acute phase, which the mass protests are, was attempted in this study.

2 THEORETICAL BASES OF SIMULATION

It is easy to see that the parametrization of mathematical tools used in physics and chemistry needs to be adjusted in relation to the social process and should be adapted to the phenomenon that is currently being considered. Processes in physics and chemistry and processes in society and politics are not the same thing. However, we will hypothetically proceed from the fact that common patterns and phenomena (threshold effects, self-organization, fractals, etc.) are spread in nature almost everywhere, and, consequently, almost the same processes (i.e. the similar ones) can be observed in society, since people are also part of nature and must obey the laws of it too. However, the question on whether the model does function properly or does not (at least in particular cases) can be answered only after a numerical experiment is over and its results (which are a short- or medium-term forecast) are compared with what actually happened.

From a mathematical point of view, social and political processes are not what can be detailed and completely characterized by a set of parameters, since the latter undergo constant changes and deformations. Here, the analogy with Brownian motion seems to be close enough: it seems that a single particle moves by well-defined trajectory, but only before it is examined more closely (Hołyst et al., 2000; Petukhov et al., 2020; Petukhov and Kaminchenko, 2021; Petukhovm 2021): the real shapes of the tracks turn out to be tortuous and nonlinear. These smaller changes in motion (trajectory fluctuations) are influenced by closer and smaller particles (molecules), which, randomly moving nearby a large particle, correct the trajectory of its movement. In social processes, such fluctuations are caused by manifestations of the free will of its participants, as well as by other accidental environmental influences. The next step in developing such a model should be to consider external influences that are not accidental, but external interference.

The proposed model is based on the assumption that individuals interact in society through a conditional "communication field" – h. This concept was introduced earlier (Hołyst et al., 2000), but had a different type of parametrization and other initial equations.

The necessity of introducing that concept is caused by a number of factors:

i) Any live cognitive system (which is both a society and a person) acts through exchange of information carried out through nerve impulses in the brain or in the opioid system of the cerebellum, or in the form of Internet information flows, or in any other suitable form.

ii) As follows from the above, the model of individuals' behaviour in society is directly related to the model of information exchange.

iii) That is why it is desirable to use the function of information exchange as the basis for the model.

For this purpose, the h-function has been introduced into model. Actually, this is a function of information exchange occurring in individuals' medium. But from a mathematical point of view, this function is to be considered as an informational field created by any person in society, which modulates the information interaction itself.

Also, from the point of view of the physical and mathematical description, it should be borne in mind that here we are talking about a society that cannot be attributed to a separate object in spatial topology, as it happens in classical physics. Indeed, from the point of view of information exchange between individuals, social space should combine both classical spatial coordinates and additional specific parameters and features. This is due to the fact that in the modern information environment there is no need to be physically closer to the object of influence in order to transmit information to it.

Thus, society is a multidimensional socio-physical space that models the ability of one individual to cover another with a personal communicative field, i.e. to exert an informational influence on him, change his parameters and the ability to move in this space. And, thus, the mutual position of those who act in this space also models the level of relationship between them and involvement in the exchange of information.

From the point of view of modelling, the conflict control by means of external influence or any other way of mediating it (Dahrendorf, 1965) may be represented as an additional function that depends at least on the spatial coordinate and that affects overall stability of the social system and structure of the last one. There are a number of analogies acting in physical systems, for example, the dissipative function, which can appear and work by a number of ways depending on physical conditions (Hołyst et al., 2000).

2.1 Monolayer Theory

The Langmuir Monolayer Theory (LMT) is one of the most successful theories describing the behaviour of separate molecules on the plane (or at the interface), as well as their influence on each other upon concentration increasing. It describes well the physical and chemical properties of *2D* systems, taking into account the cooperative interaction of molecules in them. However, before using the LMT mathematical tools to describe the processes under study, it is necessary to briefly explain its physical meaning and draw an analogy with the phenomena under study.

Monolayers on the aqueous subphase, which are the films at the air/water interface constructed of amphiphilic compounds with a thickness of just one molecule, have a special structure and exhibit unusual physical and chemical properties (Arslanov et al., 2022). Depending on number of molecules the monolayer is formed from, it can be sparse or tightly packed. The thermodynamic properties of the film are usually studied using a Langmuir device. It consists of the following elements: a "trough", which is a container filled with aqueous subphase; movable barriers designed to change the surface water area; and a Langmuir film balance with a Wilhelmy plate for surface tension measurement (Moehwald and Brezesinski, 2016). In order to determine the thermodynamic parameters of a monolayers, Irving Langmuir has introduced the concept of surface pressure which is the mathematical difference between the values of surface tension of pure water and that with the surfactant present. In addition, surface pressure is a two-dimensional analogue of common thermodynamic pressure; that is the force acting on the unit length of the measuring plate. Knowing exactly the amount of substance placed on the surface and, consequently, the number of "floating" molecules, it is possible to build the so-called monolayer compression isotherm by smoother changing the water surface area (using movable barriers). The isotherm represents the dependence of the monolayer surface pressure ($\boldsymbol{\pi}$, *mN/m*) on the water surface area available to each molecule ($\boldsymbol{A}$, Å^2). Analyzing this function (insert in Fig. 1), it is possible to make conclusions about the processes occurring in the monolayer, such as interaction of molecules, their reorientation and conformational rearrangement, as well as about phase transitions in the film.

If the area provided to one molecule is large enough, the molecules do not interact with each other, and the system as a whole can be represented as a two-dimensional ideal gas (see Figure 1a), which conforms the equation:

$$\pi A = kT \tag{1}$$

This equation is a two-dimensional analogue of the Mendeleev and Clapeyron equations for two degrees of freedom for translational motion of molecules.

When the surface area becomes too small and, consequently, the pressure increases, equation (1) stops working properly, and behaviour of monolayer can be described with a certain accuracy by two-dimensional analogue of Van-der-Waals equation:

$$\left(\pi + \frac{a}{A^2}\right)(A - b) = kT \tag{2}$$

Here the coefficient $\boldsymbol{a}$ is introduced for correcting the pressure reduced due to interaction of amphiphilic molecules with each other. This interaction consists in dispersed attraction of hydrocarbon chains, accompanied by Coulomb repulsion of charged carboxyl groups. The coefficient $\boldsymbol{b}$ corresponds to

minimum value of area per molecule in a tightly packed monolayer.

An increase in pressure transforms the monolayer into a two-dimensional liquid state, in which the molecules come close enough to interact with each other, but there is still no definite order in the film structure (Fig. 1, b).

By reducing the surface area available per molecule, the monolayer is first converted into a liquid crystal phase, and then into a two-dimensional solid state (Fig. 1, c and d, respectively). Hydrocarbon

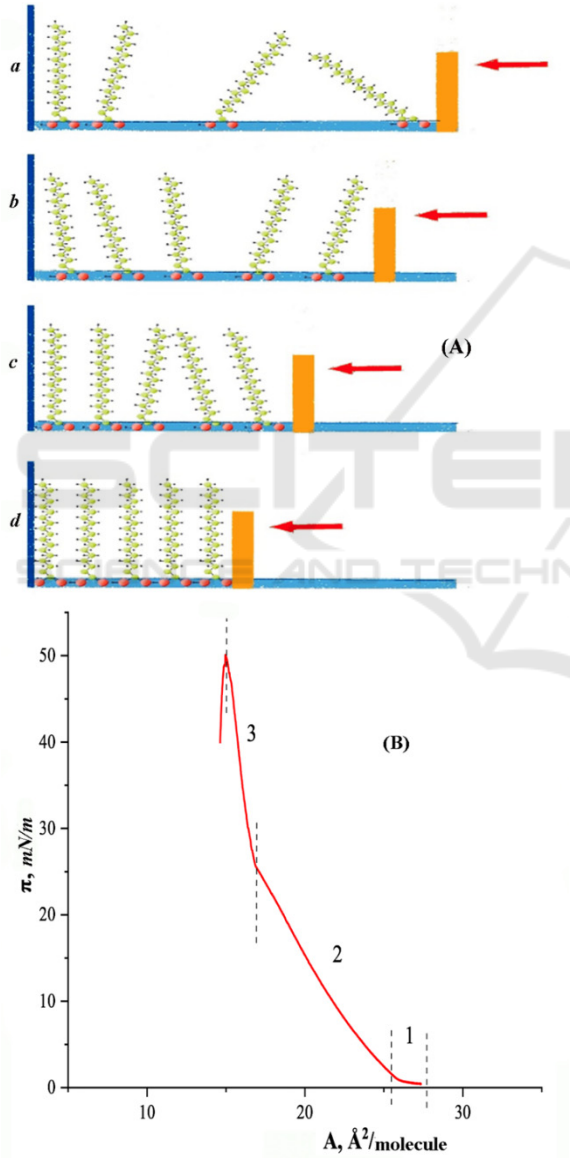

Figure 1: (A): States of phase in monolayer of stearic acid at various surface pressure: 2D gas (a), 2D liquid (b), liquid crystal (c), 2D solid state (d). (B): An isotherm of stearic acid compression at a temperature of 20°C.

chains become less flexible and line up almost perpendicular to the surface. Such transformations are phase transitions of the first kind. Further limitation of the subphase surface and, consequently, reduction of the monolayer area is accompanied by a rapid increase in pressure. As a result, the system, previously structured in two dimensions, breaks down, being unable to withstand such a load (Figure 1). So called collapse of the monolayer occur. The structure loses its integrity: one part of the molecules moves into the water, while the second begins to crawl on top of each other, forming both regular multi-layered ensembles and disordered aggregates (Oliveira et al., 2022).

Until now, the physical aspects of phase transitions in monolayers, placed on the surface of water, have not been well studied, and there is still no numerical theory explaining the multilevel supramolecular interactions of amphiphilic molecules with each other, as well as with subphase molecules.

From a chemical point of view, in order to combine all the influencing factors into a single system, this is necessary to take into account the following phenomena: steric repulsion and dispersion attraction of hydrocarbon chains; Coulomb and dipole-dipole interaction between polar fragments of molecules; formation of two-dimensional hydrates and hydrogen bonds between surfactants and water; changes in the structure of the aqueous layer surface affected by monolayer; and so on. Moreover, the introduction of ions (regardless on the charge sign) into the subphase should drastically change the potential of the double electric layer at the air/water interface, affecting the thermodynamic properties of two-dimensional phase transitions and phase states. In this regard, approximate calculation methods are currently mainly used, such as the mean field method, the scaling method and other approaches, including the Monte-Carlo method, grid models and other microscopic approaches (Lösche M. et al. 1985).

It is important to note here that a number of interesting phenomena are observed in such systems, including threshold effects associated with the processes of collapsing, self-organization of molecules (clustering), etc. These effects are of interest as they are the analogues of processes occurring in a crowd, for example, during mass riots, protests, etc., i.e. when previously unorganized crowd begins to organize itself to give separate groups and leaders appearance, or when a relatively peaceful protest goes far and destructive actions occur (threshold effect, collapse). Of course, these are the cases when protest has no serious preliminary preparation, being just spontaneous one.

3 MATHEMATICAL REPRESENTATION OF THE SYSTEM

Within the framework of this study, a type of mathematical simulation based on concept of monolayers' behaviour in liquid and liquid-crystal state is used. Here, the hydrophobic parts of amphiphilic molecules can be considered as elements of the individual's communication field. The phase transition from the *2D*-gas state to that of *2D*-liquid corresponds to process of information exchange between separate individuals or groups of them. The absence of interactions itself is out of interest for this study since the complete individuals' isolation is an analogue of monolayer's two-dimensional gas state. Thus, the transition from communication to the unification of individuals into groups (the liquid crystal state of a monolayer) is the first phase transition that is the subject of further research. Also here, the general alignment of molecules in similar spatial positions (Fig.1. b-d) can be interpreted as mutual coordination of communication fields, that is, a certain alignment of the general information in the crowd (coordination of requirements, alignment of position, self-organization).

Of most interest is the simulation of the second phase transition., i.e. from liquid crystal state to that of crystal lattice. Exploration of this process may help to predict the maximum social stress, after which the system goes to self-organization. Of the greatest interest are also cases when self-organization (crystal formation) is localized in defined areas or even points, but has not yet spread over the surface in whole. At the same time, it is worth noting once again that to solve this problem a lot of resources are required and, as to numerical methods, at present there are only partial solutions based on them, and a complete analytical solution is still not available.

At the first stage, we will limit ourselves by developing a model with a single-phase transition (from a liquid state to a liquid-crystal state) and consider it in context of conditions for consolidation of a part of society (or a protest crowd) into well-structured groups.

To perform the simulation procedure, it is necessary to set the parameter ***h***, which corresponds to radius of the communication field, and ***b***, which represents the radius of a person's personal space. If ***p*** is taken as a measure of social tension, then equation (2) can be transformed as follows:

$$p = \frac{TA^2 - hA + hB}{A^2(A-b)} \quad (3)$$

where *T* parameter (acting as the temperature factor (*kT)* in initial model) is a measure of social activity of individuals, i.e. the ability of individual to undertake a socially significant action.

When individuals (or any related elements) come each other at a distance less than ***h***, they unite and form an "island" with an area equal to ***bn***, where ***n*** is a number of individuals in group. Using a chemical analogy, the situation can be represented as a tightly packed layer. In the future, it is planned to explore various structures of such systems, which can be oligomeric, dendritic and insular. From the point of view of social sciences, this means the emergence of various types of associating the individuals into groups.

With this approach, the pressure will gradually increase with decreasing area, the trend will be similar to 1 /x (when moving along the *x* axis), but there are sharp changes caused by formation of the groups, followed by releasing spaces for residual actors.

It is important to add that in this model the process of reducing the monolayer area (leading to pressure increase potentially explainable by use of appropriate thermodynamic function analogue) is interpreted as two factors:

i) *The indoor influence* which is the growth of social tension due to internal processes in crowd (so called "massing" effects in classic researches by Lebon and Moscovici).
ii) *The outdoor influence*, i.e. provocation, incitement, etc. (or at least part of such external influence, which can be interpreted as temperature factor).

These factors may work together or separately and are to be the subject for further investigation.

Bearing in mind the above, expression (3) should be corrected. The parameter of surface area ***A*** works as a function of the two-factor parameter ***u,*** which is a measure of social tension, and, as a first approximation, a circular distribution equation can be used:

$$A(u) = \pi(R_0 - u)^2 \quad (4)$$

where R_o is the initial value.

The number of individuals, ***N*** (or the number of particles in the chemical model), is randomly distributed over this surface. Each individual occupies an area that is part of the whole surface and under normal conditions, i.e. when the local tension is lower than its threshold value, corresponds to parameter ***h***, which is the relative comfortable social

distance. When the strain exceeds, this parameter changes drastically. As mentioned above, at the first stage we will consider the transition to a tightly stacked layer. This means that area occupied by a single person will change to $\boldsymbol{b}$, which is the minimum area occupied by compact structure:

$$S_{act}(u_{local}) = \begin{cases} \pi h^2, u_{local} < u_{crit} \\ b, u_{local} \geq u_{crit} \end{cases} \quad (5)$$

The local intensity of u_{local} depends on concentration of actors on the mutual surface area:

$$u_{local}(r) = P \sum_{i=0}^{N} f_{inc}(R_{interact}, r_i, r) \quad (6)$$

where P is the proportionality coefficient,

$R_{interact}(T)$ is the distance from selected point $r(x, y)$, which characterizes the maximum radius of interaction (the average path length during Brown motion of the particle) and depends on measure of social mobility T, $r_i(x, y)$ are the coordinates of the actor i, and the f_{inc} is function which can be written like this:

$$f_{inc}(R_{interact}, r_i, r) = \begin{cases} 1, |r - r_i| \leq R_{interact} \\ 0, |r - r_i| > R_{interact} \end{cases} \quad (7)$$

And finally, the model itself may be represented as the following:

$$p\,(u) = \frac{TA^2 - hA + hS_{act}}{A^2(A - S_{act})} \quad (8)$$

When appropriate parameters for this simulation are well set, the model can be used to assess and analyze critical phenomena in order to maintain the stability of social pressure under random initial distribution of individuals. It still requires further refinement since it does not consider the structure of compact connections between actors. Such structures can be simulated with use of well-designed methods of fractal theory, and the processes occurring inside them can be described in terms of theory of percolation (Koposov and Iudin, 2008). When local intensity parameter $\boldsymbol{u_{loc}}$ changes, these structures can undergo the transformations from sparse state to tight one. Here, the compact monolayer formation is concerned as the terminate phase, after which the destruction of the particles themselves (representing individuals in given model) begins. This can be interpreted as terminal level of protest followed by acute conflict, leading to collisions and human casualties

4 CONCLUSIONS

The social hyper-clasterization of society, the sharp separation in the informational and social environment of individuals, as well as cultural and interethnic disunity, creates conditions for social conflicts and subsequent protests, riots, etc. Prevention of social conflicts, determination of their threshold conditions and search for the most effective scenarios for their suppression is an important task of modern social sciences.

In this article, the main approaches to modeling social processes were briefly considered, and a formalized definition of parameters describing the dynamics of mass protest processes was given.

A mathematical model based on the chemical theory of Langmuir monolayers and the coupling field parameter h is proposed. In addition, the basic equations are given, the interpretation and adaptation of the obtained formulas for social phenomena are proposed, and the main effects in the processes under study are described.

The next step planned for refinement of the model will include its approbation based on a numerical experiment in order to compare its results with data on real protest processes.

ACKNOWLEDGEMENTS

The research was carried out with the support of the Expert Institute for Social Research (research projects in the form of a state assignment, in the field of socio-political sciences, competition 2024).

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