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To cite this article: A D Tolstoy *et al* 2018 *IOP Conf. Ser.: Mater. Sci. Eng.* **327** 032056

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Synergetics of hardening construction systems

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Abstract. The study of hardening high-strength systems indicates the relation between the potential of synergetics and issues related to structure formation of aggregates produced on the basis of rationally selected construction mixes.

The paper considers challenges of the general principles of synergetics and sustainable development of open dissipative systems and their use in industry, as well as their understanding as complete self-regulating nonequilibrium systems. The main objective of the study was to demonstrate that the principles of self-regulating systems development can be applied in construction technology.

1. Introduction

In 1996, Russia adopted the Concept of transition to sustainable development, according to which one of the main directions of sustainable development is development and implementation of highly efficient automatic manufacturing technology and evidence-based methods to obtain new materials.

One of the main objectives of sustainable development strategy is to develop ways and means that would ensure proper adjustment to the global changes in the country. The concept reflects the right of every individual for positive environment and viable life in harmony with the environment. According to this concept, sustainable development is understood as the stable social and economic development, which does not violate its natural background. In Russia, the concept of sustainable development implies transition to practical solution of production tasks, thus preserving favorable environment and improving the quality of life [1, 2].

The development of a modern complex and other innovative technologies accelerates scientific and technical progress in the field of construction. Scientific studies aimed at development of technologies that would ensure optimal harmony with requirements of modern construction become ever more urgent.

Such scientific studies are inextricably connected with the application of new ideas and approaches to the theory and practice of modern materials science in respect of explanation of processes and phenomena of structural changes, properties of materials and phase transitions.

Many scientist from various fields of knowledge refer more often to provisions and definitions of the Haken's synergetics (the term "synergetics", which is commonly understood these days, was introduced in 1977 by Haken G., a professor of the Institute of Theoretical Physics in Stuttgart, Germany) [3]. Synergetics as a cross-disciplinary science that studies changes of a material composition and structure on the basis of self-organization principles was described in more detail in works by Prigozhin I., Zabusky I., Knyazeva E.N., Kurdyumov S.P., Ivanov V.S., et al. [4-8]. It serves



as a metascience covering and developing the general tendency of those regularities and dependences, which other sciences consider as part of their concept. The synergetic method acquired the status of a general scientific method and is widely used in modern science. Many scientists note that synergetics is a paradigm of modern, post-classical science. Its categorial component (bifurcation, fluctuation, dissipative structure, synergetic effect, etc.) allows analyzing changes of various open, nonequilibrium, and complex systems.

2. Application of principles of synergetics in explanation of structure formation of artificial stone hardening.

The objective of the study was to demonstrate the possibility and validity of applying (or, if possible, implementing) the principles and concept of synergetics to explain processes of structurization of artificial stone hardening on the basis of a rationally selected multicomponent mix.

This approach to the study of materials science problems has not been yet developed enough in scientific literature. The following key factors contributed to the decision on applying the synergetic method:

1. The basic postulate of synergetics is the fact that the application of synergetic principles is not clearly defined and thus cannot have certain frameworks since it covers all fields of natural sciences.
2. The compliance of multicomponent hardening systems to basic concepts and methodological aspects of synergetics that represent complex, nonequilibrium, evolutionary systems with dramatic and fast formation of new microscopic (local) growths and appearance of new properties of a system.
3. The system of the hardening mix is open and far from being the thermodynamic equilibrium, where the main principle of self-organization includes identification of a new order and a new structure through chaos due to the content of a large number of interrelating elements.
4. The hardening system ensures metabolic action and energy exchange with external environment thus leading to regularity and self-organization.
5. A fundamental mechanism of synergetics, i.e. a bifurcation mechanism, in which the bifurcation point, being the most sensitive state to insignificant “excitations”, “violations” (fluctuations), is considered as the mixing with water, after which the system “chooses” the most optimal way of development, i.e. hardening, strength gain and transformation into a calculous body or, in other words, transition to a new attractor.

The thermodynamic approach to self-organization can be seen at the Belgian school of I. Prigozhin [4]. This school replaces the Haken’s concept of synergetics that includes understanding of a structure as a state resulting from coherent (coordinated) behavior of various particles with the concept of a dissipative structure. In open systems, which are in the process of exchange with environment by energy or substance flows, a uniform equilibrium state can lose the stability and convert irreversibly into the non-uniform steady state, which will remain stable in relation to small excitations. The content-related definition of the thermodynamic system as a complex of multiple units of structural particles interacting among themselves (atoms, molecules, etc.) defines statistical regularities allowing characterizing the state of a system by a small number of parameters. Thermodynamic systems tend to interact both among them and with the environment through energy and/or substance exchange. Depending on the nature of interaction with the environment, thermodynamics considers several types of systems. The system, which is deprived of substance and energy exchange with the environment, is isolated. The system exchanging only energy with the environment is closed. Finally, the open system is the system that ensures energy and substance exchange with the environment.

In terms of their structure, thermodynamic systems can be divided into homogeneous and heterogeneous. Systems, which properties change continuously spatially, are called homogeneous. In a particular case, the properties of any component of uniform homogeneous systems are identical. The heterogeneous system includes several uniform or homogeneous parts with peculiar properties. Thus, the properties of heterogeneous systems change stepwise upon transition from its one homogeneous part to another. A homogeneous part of the heterogeneous system, which is separated from other parts, is called a phase. Examples of the heterogeneous system are systems consisting of coexisting phases of

one or several individual substances. The thermodynamic approach implies that the condition of a thermodynamic system is defined by setting a number of macroscopic parameters (volume, pressure, concentration, etc.) as well as state parameters characterizing various conditions of a system in general (internal energy, enthalpy, entropy and free energy – Gibbs energy). Due to this, the thermodynamic approach is very similar and can be applied to the majority systems – physical, chemical, biological, etc.

The energy of the thermodynamic system possesses energy that consists of a large number of particles (atoms, molecules, etc.), which are constantly moving and interacting among themselves, as well as with bodies surrounding the system or physical fields created by the environment. The energy of a system, except for its external component, i.e. kinetic energy of a system as a unit and potential energy of a system in the field of external forces, is called internal energy of a system. It is essential that for thermodynamic systems, the internal energy serves as an extensive parameter. Systems, the internal energy of which is not linearly dependant on the number of particles, cannot be described by thermodynamic methods [9].

In terms of limits of thermodynamic approach applicability, they are defined by postulates of thermodynamics. The postulate on thermodynamic equilibrium, which is the first postulate of thermodynamics, says that with time any isolated macroscopic system transfers into the condition of thermodynamic equilibrium and cannot leave it spontaneously. In turn, irreversible and spontaneous transition of the isolated system to the condition of thermodynamic equilibrium is a common fundamental property of all macroscopic objects. Quite a significant number of states, which replace each other during dynamic evolution of a macrosystem, among which, along with microstates corresponding to thermodynamic balance, there are microstates which clearly correspond to various thermodynamic nonequilibrium macrostates. Hence, thermodynamics describes not only the equilibrium states and their properties but also some regularities close to equilibrium. The second postulate is the postulate concerning temperature. It states that any macroscopic system, being in the condition of thermodynamic equilibrium, is characterized by a special intensive thermodynamic parameter – temperature, which is uniform for all parts of a system and defines its state together with other macroscopic parameters. It turns out that the equality of temperatures of two or several systems is a necessary condition of their thermodynamic equilibrium [10].

An important conclusion on equilibrium and temperature is that in the condition of thermodynamic balance internal parameters of a system, as well as the internal energy of a system, are functions of external parameters and temperature. The third postulate is that the temperature of an equilibrium system increases with the increase in its internal energy, for example, during energy transfer from surrounding bodies. Transitivity of equilibrium state allows comparing temperature of various equilibrium systems, making their thermal contact comparable with a reference body, which serves the temperature detector.

For example, let us consider the system of chemical kinetics equations, which describes a unique situation: a thoroughly studied mechanism of m-phasic reaction (m – number of elementary acts) with n-number of substances. The algorithm of a dynamic system is clearly defined by the reaction scheme.

The reaction behavior can be foreseen through the calculation of the free energy (Gibbs energy).

Gibbs energy (Gibbs thermodynamic potential, free enthalpy) – the function of a system state (*G*) defined from the expression:

$$G = H - TS, [\text{J or J/mol}]$$

where *H* – enthalpy (heat content), J/mol;

T – absolute temperature, K;

S – entropy, J/mol.

There is a certain rule in this method: all spontaneous processes are followed by the reduction of the Gibbs energy prior to achieving the minimum corresponding to the equilibrium state of a system (Fig. 1).

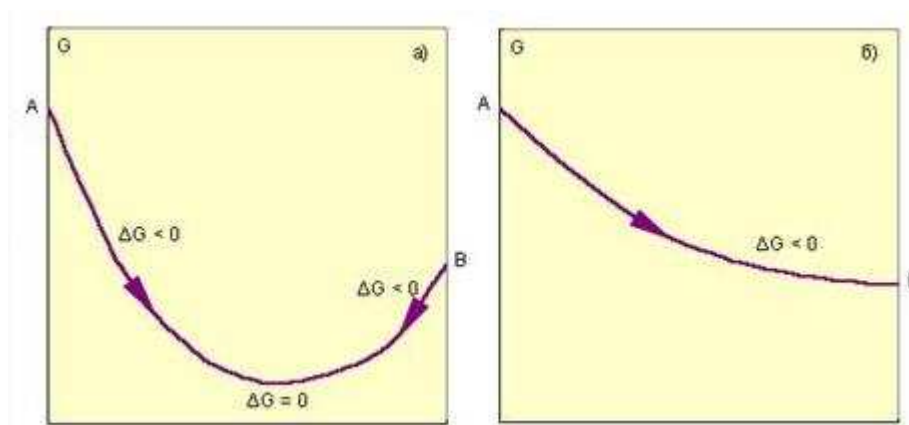


Figure 1. Change of the Gibbs energy: *a* – reversible process; *b* – irreversible process

This parameter of a state is used in mathematical calculations, since the decrease of the Gibbs energy in the equilibrium process (at constant pressure and temperature) is equal to the maximum useful effect [11-14].

The formation of hydroaluminates, hydroferrites and hydrosulfoaluminates of calcium, portlandite, amorphous aluminum, iron and gypsum hydroxides (Tab. 1) as products of the reaction is considered in thermodynamic analysis $\text{CaO}-\text{C}_3\text{A}(\text{C}_3\text{F})-\text{Ox}-\text{H}_2\text{O}$ in normal conditions.

Thermodynamic stability of calcium hydroaluminates and hydrosulfoaluminates at increased temperatures was analyzed according to the calculated Gibbs energy. The obtained results show that up to the temperature of 348.15 K, associations of calcium aluminate trisulfate hydrate with gypsum (reactions 1, 2, Tab. 1) are thermodynamically steadier products of the reaction. At a temperature above 348.15 K, the absolute Gibbs energy of this reaction decreases, which indicates the unstable state of $\text{C}_3\text{FCs}_3\text{H}_{32}$ in these conditions with its transition to calcium monosulfohydroferrite and formation of two molecules of calcium sulfate dihydrate (reaction 3, Tab. 1).

Table 1. Change of the Gibbs energy and volumes of products in hydrate formation reaction in hardening systems

No	Chemical equation	ΔV solid phase		ΔV condensed phase		$-G_{298}^0$ reaction, kJ/mol
		cm^3/mol	%	cm^3/mol	%	
1	$\text{C}_3\text{A}+3\text{CsH}_2+26\text{H}_2\text{O}=\text{C}_3\text{ACs}_3\text{H}_{32}$	311.83	128.72	-67.13	8.60	235.94
2	$\text{C}_3\text{F}+\text{Ca}(\text{OH})_2+3\text{CsH}_2+25\text{H}_2\text{O}=\text{C}_3\text{FCs}_3\text{H}_{32}$	398.59	123.46	-51.91	6.71	107.07
3	$\text{CsH}_{0.5}+1.5\text{H}_2\text{O}=\text{CsH}_2$	21.43	40.60	-5.60	7.02	4.60
4	$\text{CaO}+\text{H}_2\text{O}=\text{Ca}(\text{OH})_2$	15.23	90.82	-2.68	7.68	55.90

Thus, the calculations demonstrate thermodynamic preference of formation of associations of aluminum- and ferrous calcium trisulphate hydrate at normal temperature and transformation of At-phases into to calcium monosulfoaluminate at increased temperatures.

The obtained results make it possible to manage the process of interaction in a hardening multicomponent system with cement thus changing the oxidizing capacity of a system.

3. Conclusions

The synergetic approach to hydration and application of a thermodynamic method makes it possible to manage structurization of hardening systems. This approach also allows analyzing the condition of basic structural elements of the open metastable system of hardening multicomponent concrete. It is also possible to define indicators of process completion in a nonequilibrium system with fixing a new state – from plastic to calculous state, i.e. transition to a new attractor. These definitions accurately explain the mechanism of hydration and clearly correlate with synergetics. The object of further study includes identification of a role of each component within the multicomponent high-strength hardening system on the basis of their thermodynamic parameters taking into account synergetic principles.

4. Acknowledgments

The paper is prepared in the framework of the Flagship University Development Program at Belgorod State Technological University named after V.G. Shukhov using facilities of High Technology Center of BSTU named after V.G. Shukhov.

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