2017 Water Reactor Fuel Performance Meeting
September 10 (Sun) ~ 14 (Thu), 2017
Ramada Plaza Jeju • Jeju Island, Korea

PRINCIPLES OF MODELLING OF TECHNOLOGICAL PROCESSES

M.A.Shustov, I.I.Loktev, A.V.Strukov, E.A.Milchakov, E.V.Vichodcev

B.Khmelnitsky str., Novosibirsk, Russia, 630110, loktev@nccp.ru, *PJSC NCCP of Fuel Company TVEL, State Corporation ROSATOM*

ABSTRACT: *Good understanding of all technological factors and conditions, influencing achievement of necessary quality characteristics of nuclear fuel, plays important role for providing high fuel performance in reactor. There are additional restrictions on production of nuclear fuel, which impose requirements of economy, ecology, safety, productivity and control of process of production and must be taken into account. Technological researches which proceed continually includes different science methods - statistical, pilot and theoretical studies. One of them, most effective, is modeling, which gives evident, applicable for the organization of faultless production, results. In this report examples of the general and concrete models of technological processes which can be used during the carrying out technological researches and development of new productions are given.*

KEYWORDS*: transmitting functions, structural - operational model, phase space, packing models, cellular automation model, model of material balance, model of technological trajectories.*

I. INTRODUCTION

Process of production of an industrial output can be simply presented in a general flowchart as consecutive (step by step) transformation of an initial product into finished goods with a necessary set of technical characteristics. Production is carried out on production lines in which next streams are organized in mutually concordant view: material, power and information (*Ref. 1*). Information can be of kind: controlling, operating and registering. A state of a product on various stages can be characterized by parameters of one or some various structural levels of the product. It is possible to show the described production line as a scheme of Fig. 1, where to A_i - separate operations, B_i a state of a product after *i*-operation. Operation can influence the separate structural level, or some of them.

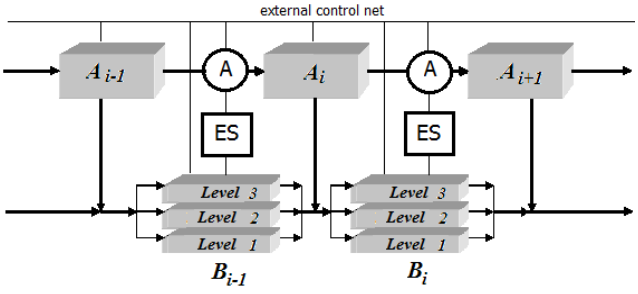


Fig. 1. Scheme of smart-production.

A smart-technology with internal and external control can be made for well-studied production line. In the scheme of Fig. 1 *ES* - elements of artificial intelligence with the built-in software which contains model of operation and the principles of regulation of the modes of its performance, and also is available the network of external correction which is adjusting at one moment all sites of the scheme is shown.

However, despite high technological level of production of modern fuel for nuclear power plants, technological capabilities are limited to reasons of cost, safety, the ecological acceptability, competitiveness. These factors is of particular importance for new types of fuel (tolerant fuel, fuel for reactors of the fourth generation), which have, as expected, multi-component structure. There are two groups of significant factors from the point of view of behavior of this fuel in the reactor: influence of components on achievement of required operational characteristics of fuel, and also residual uniformity of distribution of these components at production of fuel by chosen process. One of important operation of this process is pressing of pellets.

Modeling of technological processes allows defining their limit opportunities and level of their acceptability, helps to estimate role of technology factors on providing of design characteristics of ready fuel. A number of examples of such models stated in a generalized view are given in this article. They are structural and operational model (II.A), model of technological trajectories (II.B) - from point of view of the first group of significant factors. The model of packing of dispersive materials (II.C), mixing models (II.D.1; II.D.2) - the model of final elements (II.E) and model on the basis of material balance (II.F) - the second factor group, factors of uniformity.

II. DISCUSSION OF SOME TECHNOLOGICAL PROCESSES MODEL

II.A. Structural - Operational Model

Operational properties of fuel are characterized by the parameters defining its state at the different structural levels (pore and grain distribution, composition, nonintegrated formations, density, geometry). At different stages of technological process of production, and then at stages of life cycle these properties undergo certain changes, but they define temperature of pellet, dimension stability, gas release and so on. The full scheme of interactions of such factors is submitted by structural and operational model (in general).

The scheme on Fig. 1 is a structural and operational scheme. All process in regarded Structural and Operational Model would be result of processes at all structural levels of system at consecutive course of all operations and therefore can be presented by double product of all private operators of levels on separate operations and all operators of operations of separate structural levels. It would not give particulars about structure of a studding object, but will help to establish this interrelations with the next operations, which can be expressed by operators. These operators should be presented by transmissive functions, transformation actions, not only on nearly, but on all another structural levels of object. The scheme in Fig. 1 can be presented by Table 1 in the descriptive form.

TABLE 1. Table of multilevel state

Material	Process	Level 1	Level 2	Level j	Level j+1	Level m
INITIAL STATE		a_{01}	a_{02}	a_{0j}	$a_{0(j+1)}$	a_{0m}
	OPERATION 1	b_{11}	b_{12}	b_{1j}	$b_{1(j+1)}$	b_{1m}
STATE 1		a_{11}	a_{12}	a_{1j}	$a_{1\,(j+1)}$	a_{1m}
	OPERATION 2	b_{21}	b_{22}	b_{2j}	$b_{2(j+1)}$	b_{2m}
STATE 2		a_{21}	a_{22}	a_{2j}	$a_{2\,(j+1)}$	a_{2m}
	OPERATION i	b_{i1}	b_{i2}	b_{ig}	$b_{i(j+1)}$	$b_{\ im}$
STATE i		a_{i1}	a_{i2}	a_{ij}	$a_{i(j+1)}$	a_{im}
	OPERATION n	b_{n1}	b_{n2}	b_{nj}	$b_{n(j+1)}$	b_{nm}
STATE n		a_{n1}	a_{n2}	a_{nj}	$a_{n(j+1)}$	a_{nm}

It is clear, that the table can be continued to the right and down to natural limits. So, process of production of fuel for nuclear power plants can consist of production cycle, burning of fuel in the reactor, unloading and burials of spent fuel.

In this chain it is possible easily to see and study, for example, impact of impurity on microstructure of fuel, on sintering process and course of neutron reactions, and also on activity of the unloaded fuel.

From another side, sintering, for example, can consist of processes on different structure levels: diffusion of atoms, creation of crystal structure, formation of grains, shrinkage of pellets, formation of batch average density and of dispersion of batch parameters. This hierarchy scheme helps trace total way of forming final fuel properties and their evolution on stages of working cycle.

All process in regarded operational and structural framework would be result of processes at all structural levels of system at consecutive course of all operations and therefore can be presented by double product, Eq. 1, of all private operators of levels on separate operations (φ_{ij}) and all operators of operations of separate structural levels (ϕ_{ij}):

$$a_{nm} = \prod_{i=1}^{n}\prod_{j=1}^{m}\varphi_{ij}\phi_{ij}a_{ij} = \Omega^{nm}a_{01} \qquad (1)$$

II.B. Representation of processes in phase space

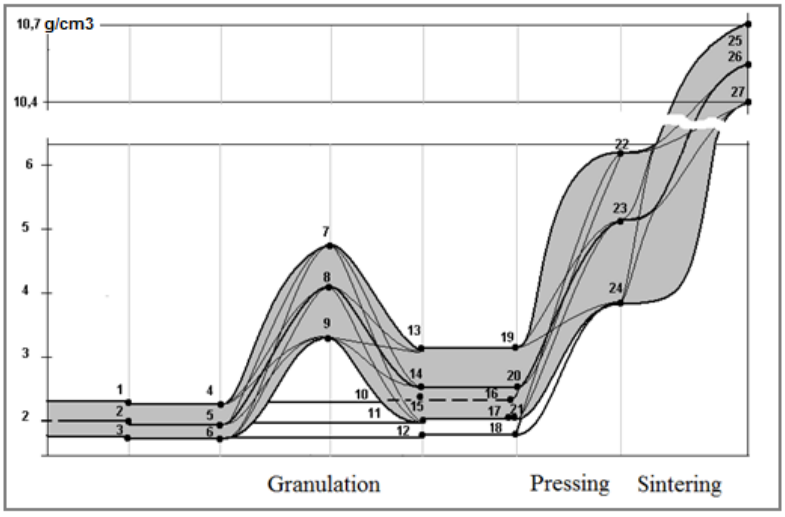


Fig. 2. Options of density change.

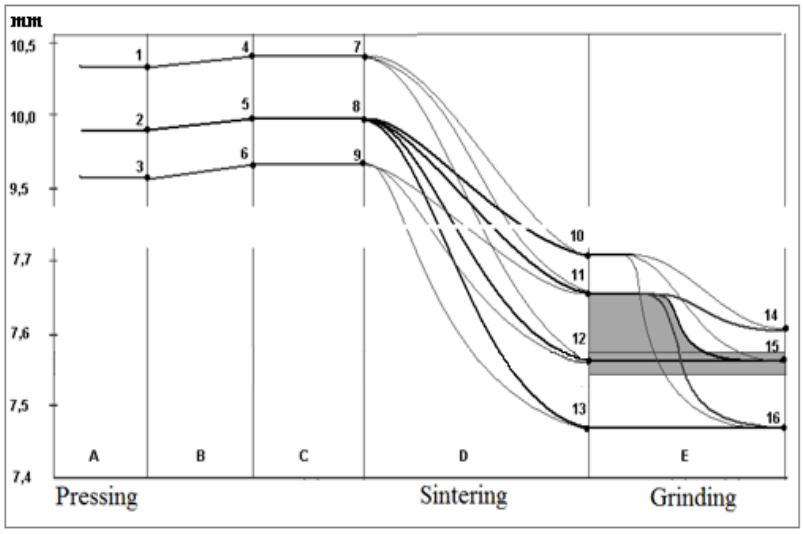


Fig. 3. Options of pellet diameter change.

Technological processes can be presented as phase transformation of initial materials. The graphical representation of process in coordinates of phase characteristics and time can serve as way of modeling. Uniform part of any material system, object of research, which state can be characterized in some time point with helping of certain set of parameters, we can name as phase. Then a technological process can be presented as phase transformation of initial materials. Parameters of

phase characteristics can be geometric parameters also. The graphical representation of process in coordinates of characteristics of phase state and of time can serve as way of its modeling. Some graphic models of the same object, which are made in different sets of coordinates, represent various projections of the studied systems and processes on the plane or space of the chosen parameters. Models with a time scale, dynamic models, can be called as technological trajectories.

Change of any parameters in scale of time is called kinetic curves, when the behavior of processes in time, or object state evolutions gradually passes from one phase state into another are studding. Two diagrams of change of diameter and density of pellets, depending on stages of their production are shown in Fig. 3 and 4 as example (*Ref. 2)*. Sequence of stages on graphic is the same as time scale.

Feature of the provided schedules is representation of all possible technological trajectories, on each technology stage. They can help developers of technology to make a final choice of the scheme of production of fuel, they present the good manual.

II.C. Particles packing models

Packing models help to understand behavior of powders during their mixing. Some of them are discussed here. At production of fuel compositions often use mixing of various materials. Prepared mixtures of powders are presented themselves as packing systems of powder particles. Very often, particles have form, which close to sphere. Uniformity of mixes depends on sizes distribution of particles. Packing models help to understand behavior of powders during their mixing and carrying out of technological operations. Some of them are discussed in few words here.

II.C.1. Packing of mono-fractions of powders

It is known in practice that the layer of spherical particles of one size will seek to occupy about 64% of capacity volume if to settle a layer. It is not most dense packing, actually it consists of sites with various order of particle arrangement, bridges with emptiness between particles are also possible.

II.C.2. Packing of two mutual complementary mono-fractions

There is a residual volume (an empty phase) between particles in case of *II.C.1* and particles of smaller diameter getting through the layer of the first fraction could occupy it. They are named as mutually complementary fractions. Their diameters, D_1 and D_2 have to answer a formula (2), if they are spherical or formula (3), if they are non-spherical:

Spherical particles: $D_2 \le 0{,}15\ D_1$ (2)
Wrong particles: D_2 form $\le 0{,}10\ D_1$ (3)

Second phase must occupy quarter of volume of total mixture, or one third of first phase volume. The maximum packing ratio of two fractions can reaches 85-87% with parameters (diameter, volume share), answering to the principle of optimality. It is possible to receive packing ratio of 95% and more, continuing filling of empty phase with smaller complementary fractions. General formulas for it:

Conditions of suitable complementary mono-fractions: $\begin{cases} D_n = 0{,}15 D_{n-1} = (0{,}15)^{n-1} D_1 \\ v_n = 0{,}25 v_{n-1} = (0{,}25)^{n-1} v_1 \end{cases}$, (4)

II.C.3. Packing of two non-complementary mono-fractions.

A packing with rate more than 64%, but less than 87% can be received for mixtures of two non-complementary mono-fractions. It would be nearer to top or to lower limit, depending of that, parameters of mono-fractions come far or close to optimum. Using experimental and literary data, it is possible to make by interpolation method the chart of packing of two fractions with any diameter and volume relation, Fig. 4.

II.C.4. Packing of poly-disperse powders

The model of packing of powder of poly-disperse structure can be presented (Ref. 2), it use optimization of fractional composition of the powders received in the natural way, for example, by crushing. The model is based on position, derived

from Fig. 4: packing of powder mono-fraction would change no more, than 1-2%, if particle diameter scattering not be larger than 1,5. Powder can be sieved on fraction so that to consider them as mono-fractions, further it is possible to do of optimal mixture with maximum packing, using the chart in Fig. 4.

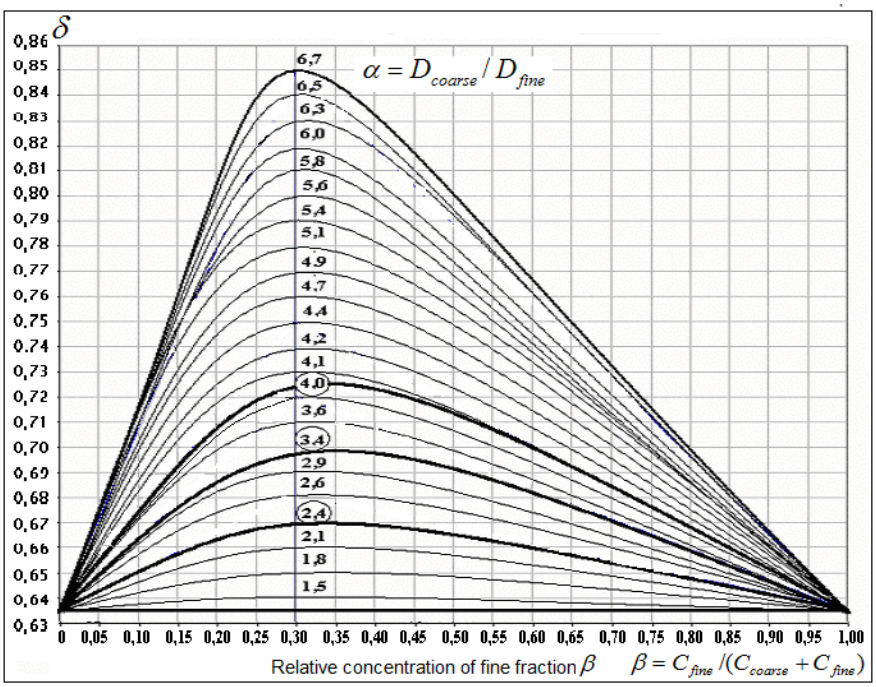


Fig. 4. Chart of packing of two any mono-fractions

II.D. Models of mixing

II.D.1. Model of powder exchanging in phase volumes

Models of mixing of powders would be presented as transitions of one and the same volume of powder from one phase volume to another. Content of this volume continually changes. This kind of model is a bright example of possibilities of phase space principle. Being not connected with any geometrical attributes of systems, the model nevertheless can correspond to essence of processes, which are occurring there.

For example, two kinds of powder, *A* and *B*, with close properties are loaded into any mixer. Let initial volumes of those powders are phase volumes up to end of process. Then mixing process would be transitions of one and the same volume of powder (part *k* of total mixture volume) from one phase volume to another, Fig. 5. At first cycle, part *k* of powder *A* is transferred into the phase volume of powder *B*, and the same volume of powder *B* is transferred into the phase volume of powder *A*. At second cycle, the same part *k* of transferring powder *A* will contain some part of powder *B*, which was transferred there during first cycle. So, step by step process comes to state, when concentrates of powder *A* (and powder *B*) will be the same in both phase volumes.

Conditionally this process is shown in Fig. 5. Setting different values for an initial ratio of the phases V_A/V_B, it is possible to construct family of curves for various options of performance of operation, Fig. 5.

Initial state: n=0, $C_{va}^0 = 1;\ C_{vb}^0 = 0$, First cycle: n=1, $C_{va}^1 = 1-k$; $C_{vb}^1 = \frac{ka}{b}$ (5)

Second cycle: n=2, $C_{va}^2 = 1-2k+\frac{k^2}{b}$ $C_{vb}^2 = \frac{ka}{b}\left(2-\frac{k}{b}\right)$

Final state: n≈∞ $C_{va}^{\infty} = C_{vb}^{\infty} = \frac{v_a}{v_a + v_b}$

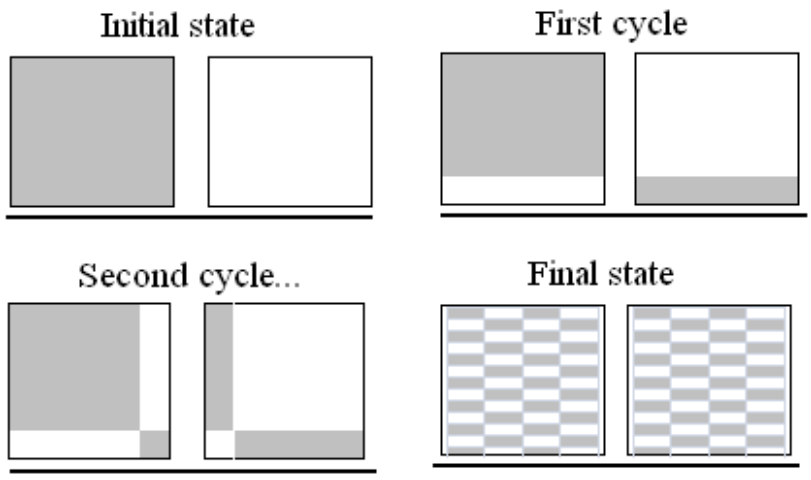


Fig. 5. Transition of phase volumes from an initial state with completely divided phases to final with uniform and identical distribution of phases in both volumes.

The general analytical formula for concentration of a cycle n does not exist, formulas become too bulky. Estimation is made by consecutive calculation on the computer for each subsequent cycle with use of the previous result.

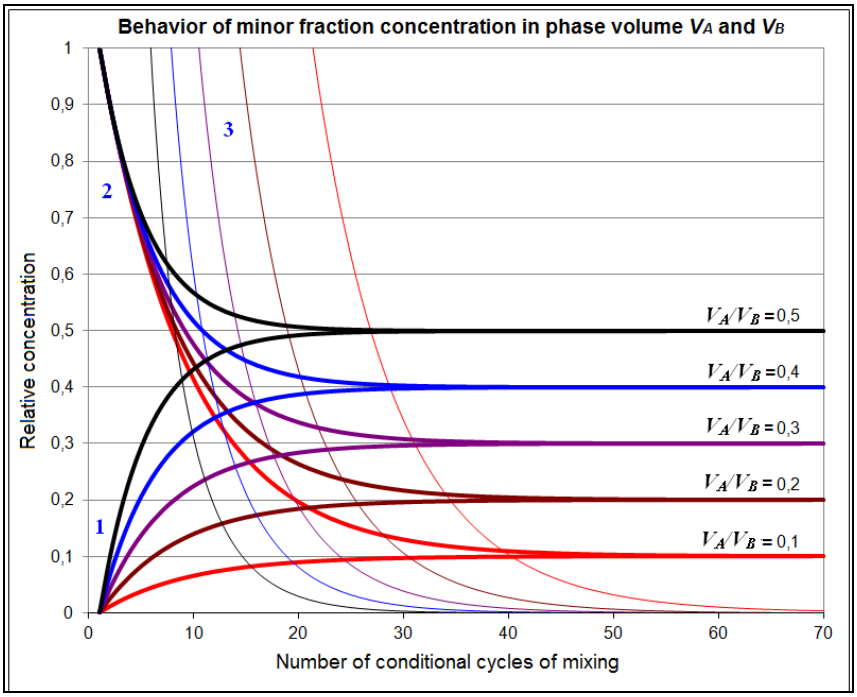


Fig. 6. Behavior of concentration of one fraction (minimal) depending on part of mixing *k*, and fraction volume relation of V_a/V_b. Three families of curves are given in drawing: 1 and 2 - concentration of a minimal phase in one and other phase volume; 3 - a difference of concentration of phases in different phase volumes.

The model is used for definition of necessary number of mixing cycles *m*, at which the set needed residual heterogeneity is reached. For assignment of the model to the real mixer it is necessary to calibrate a of abscissa axis. This model can be used in FMEA analysis in searching of compromise between technological expenses and fuel reactor performance.

II.D.2. Cellular automation model

For the description of mixing of powders with use of mixers in which particles movement is casual, can be used model of cellular automation. There is a set of approaches to the description of technological processes on the basis of application of casual processes which are describing by method of the cellular automation. Here are considerations, what of them can be used for solving problems of receiving uniform mixes.

Degree of uniformity can be defined by extremely small volume of sample, which else shows the content of ingredients of mixture, near average. Further decrease of volume will lead to fluctuations from zero to 100%. This volume of minimal sample can be named as physical limit of uniformity. It can be defined by a mixture volume, falling on one particle of smaller components. It is possible to show that when mixing two powders with a mass of M_1 and M_2, density of ρ_1 and ρ_2 the physical limit of uniformity of distribution of a minor component with a diameter of particles of *a* will be equal:

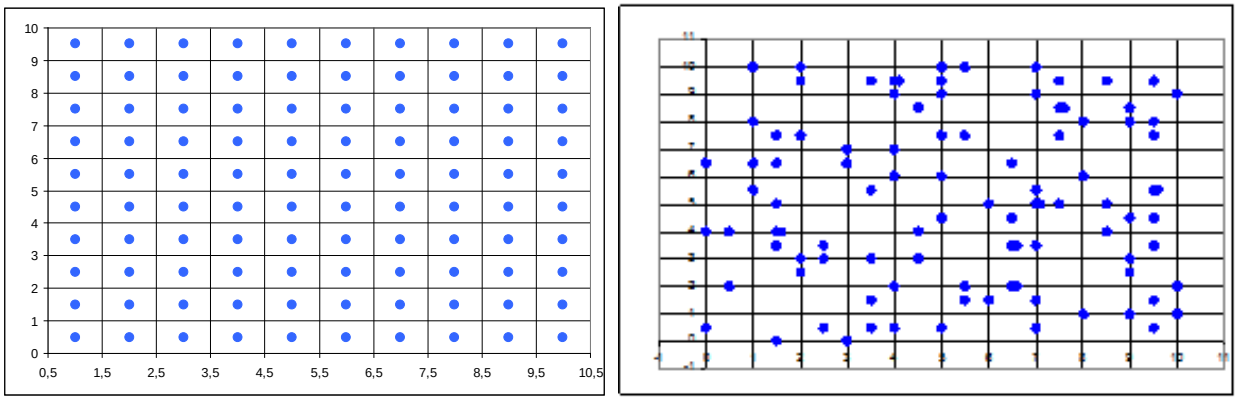
$$a = \overline{d}_1 * \sqrt[3]{\frac{\pi}{6}\left(\frac{\rho_1}{\rho_2}\right) \Big/ \left(\frac{M_1}{M_2}\right)} \qquad (6)$$

However, there is also statistical limit of uniformity. It is connected with effect of deviation from ideal homogeneity of phase distribution, if it would be in initial stage after next mixing. These fluctuations will not be great and will not be depending from time of mixing, because the number of particles and volume of mixture remain invariable, however the limit of uniformity will change. There is considering that steady state of mixture homogeneity will be the same, if mixing was from beginning of process, or after ideal distribution of ingredients. Really last case is impossible, but can be modeled.

For this purpose it can be estimated the movement of the points, which are evenly distributed on a coordinate grid 10x10, Fig. 6(a) during their displacement in the casual direction under the law (7).

$$x_n = x_{n-1} + RNDa_n = \sum_{k=1}^{n} RNDa_k \; ; \qquad y_n = y_{n-1} + RNDb_n = \sum_{k=1}^{n} RNDb_k \qquad (7)$$

After five displacements of each point, Fig. 7(b), it can be estimated average point quantity in volume of splitting, Table 2. As for the volume of splitting, it was taken as a column of a coordinate field, Fig. 7 with a width (1-5)*a*, where a - step of displacement, equivalent of the physical limit of uniformity (one point in a cell).



a) b)

Fig. 7. A coordinate field of cages with ideal distribution of points (a) and after five casual displacements on two axis (b).

Table 2. Characteristic of statistical uniformity deviations of point distribution.

Volume of splitting *a*-physical limit of uniformity	Quantity of points in volume of splitting	Scattering, %
a, ideal mixture	10	0
a, after 5 displacements	5-14, average near 10	to 50%
2*a*, after 5 displacements	7-12, average near 10	to 30%
3*a*, after 5 displacements	8-11, average near 10	to 20%
5*a*, after 5 displacements	9,6 average near 10	4%

It is shown from the table that the deviation of number of points in volume of splitting from average value decreases with increasing of the sample volume. It is possible to draw a conclusion on the basis of the obtained data, that for decreasing of statistical heterogeneity of ingredient content in mixtures to several percent, it is necessary to take sample with volume not less, than 5 volume of physical limit of homogeneity.

For the description of mixing of powders with use of mixers in which particles movement can be considered casual, the model of casual movement of a point under law (7) can be used. Trajectories of movement of points were received with model for 1000 casual steps. 5 such trajectories are shown in Fig. 8.

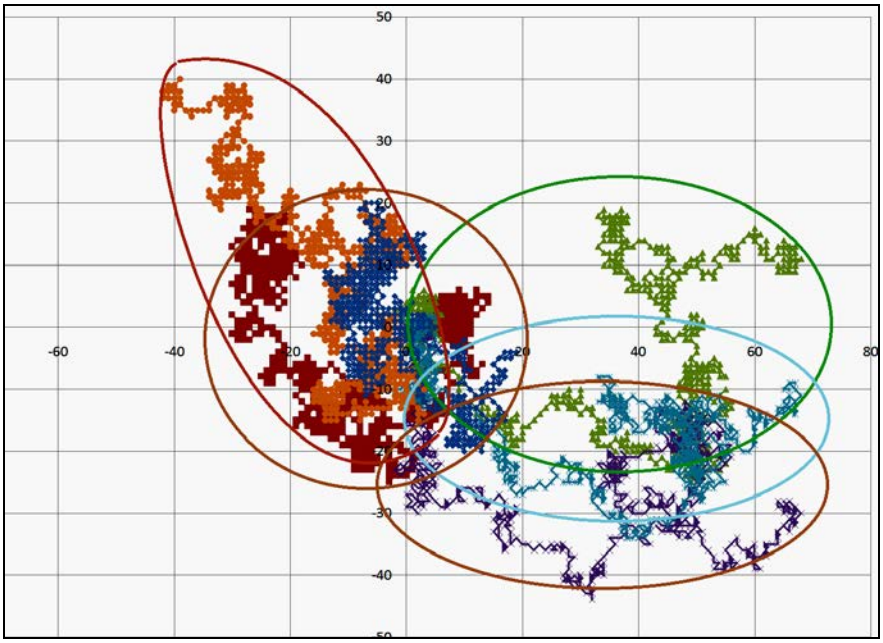


Fig. 8. Schedules of casual movement of five points on 1000 steps.

Statistical processing of movement of 10 points showed that average speed (diffusion) of points is 20 times less, than the speed of their linear movement.

If to consider that for achievement of uniformity of mixing it is necessary to create a condition under which separate particles must do m cycles and come distance, comparable with dimensions of a mixing zone l, the number of cycles n has to be meet a condition:

$$n \geq 20\frac{l}{m} \qquad (8)$$

II.E. MODEL OF FINITE ELEMENTS FOR POWDER PRESSING

To describe scheme of all forces during pressing and understand their action, can be used finite elements method (FEM). Fuel pellets during pressing are under different pressure at different places. Pressure from punch, p, create hydrostatic forces, applied to cylindrical surface of die. During movement of compressed powder lateral forces create opposite forces of friction (coefficient ξ), which relaxes punch force. Due to internal friction (coefficient ψ), external friction forces transfers its opposite action to internal column of powder. On Fig. 9 is shown pellet, spitted into finite elements and forces, acting in each of element. The model allows estimate of wedge of density, local stress, dangerous for pellet integrity due to local over pressing. For this purpose it is necessary to define experimentally coefficients of friction and dangerous density differences of green pellet.

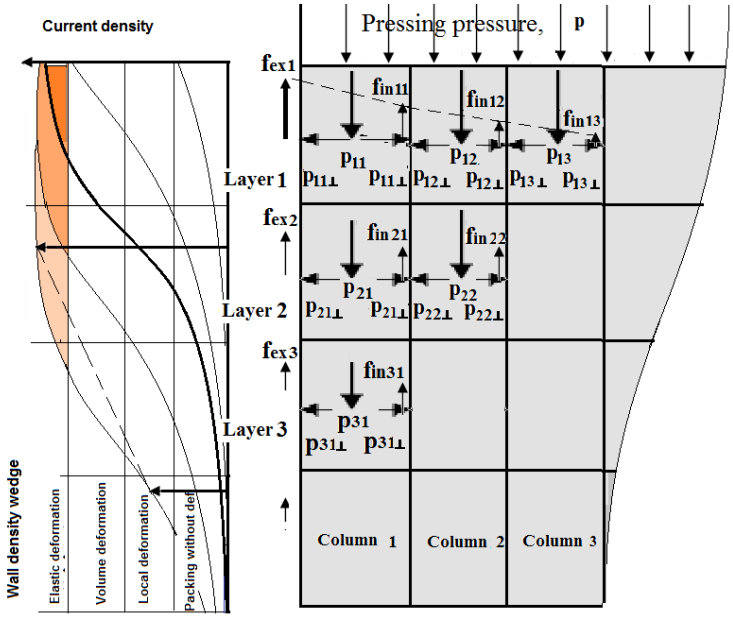


Fig. 9. Splitting a pellet into final elements, action of pressing forces in them, distribution of density

Table 3. Characteristic expressions for a column 1, Fig. 9.

Finite element	Press pressure	Transverse pressure $p_{\perp}$	External friction f_{ex}	Internal friction f_{in}
11	p_{11}	νp_{11}	$p_{11}\nu\xi$	$\nu\xi\psi p_{11}$
21	$p_{11}(1-\nu\xi)$	$p_{11}\nu(1-\nu\xi)$	$p_{11}\nu\xi(1-\nu\xi)$	$\nu\xi\psi p_{11}(1-\nu\xi)$
31	$p_{11}(1-\nu\xi)^2$	$p_{11}\nu(1-\nu\xi)^2$	$p_{11}\nu\xi(1-\nu\xi)^2$	$\nu\xi\psi p_{11}(1-\nu\xi)^2$
n1	$p_{11}(1-\nu\xi)^{n-1}$	$p_{11}\nu(1-\nu\xi)^{n-1}$	$p_{11}\nu\xi(1-\nu\xi)^{n-1}$	$\nu\xi\psi p_{11}(1-\nu\xi)^{n-1}$

II.F. MODEL ON PRINCIPLE OF MATERIAL BALANCE

In the course of technological transformation of input material a change of weight can serve as the characteristic of process if it does not change or an indicator of its stability if it does not change. If the mass of a product does not change, but its density changes, exist possibility for prediction of geometry parameters, as sum of their variations is invariable, Eq. (9),

$$\omega_\gamma + 2\omega_D + \omega_H - \omega_M = 0 \qquad (9)$$

where ω_γ - density variation, ω_D - diameter variation, ω_H - height variation, ω_M - mass variation, gives the chance of adjustment of some parameters of pellets using changes of others ones.

III. CONCLUSIONS

The organization of highly effective modern production of fuel with automation of control and management of technological processes, production of high-quality modern fuel for nuclear power plants, and also for development and deployment of industrial production of fuel for reactors of new generations, requires of deep and detailed understanding of all processes and properties of the used materials. Different kinds of modeling promote technological researches on these directions. They help find of compromise between of technological scheme of nuclear fuel production with minimum expenses, from one side, and its operational behavior, conforming to all strict requirements of successful working in modern reactor from another side. Role of modeling becomes more important for new kind of fuel, which have composite structure.

IV. REFERANCE

1. V.A.Vlasov, Tichomirov, I.I.Loktev modeling of technological processes. – Tomsk: Issue: TPU, 2006. -104p.

2) I.I.Loktev “The packing model of polydispers materials”. *Materials of 7-th interbranch meeting on reactor materials*. Dimitrovgrad 2003.