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METHODOLOGICAL PRINCIPLES OF SIMULATION MODELLING AND PREDICTION OF THE PROPERTIES OF POWDER MATERIALS

The basic principles and philosophy of simulation modelling properties of powder materials. The method of selection of mathematical models, methods display the properties of the finished product, depending on the source material. The recommendations for further use are given appropriate techniques for writing computer programs

Fig.1.

Introduction.

Powder materials are the most common for both natural and artificial. They are widely used in many industries and construction. In the structure of these materials are very diverse and heterogeneous materials properties vary as a factor structure. Therefore, to approach the problem of devising methods of mathematical modelling of structures need to differentiate each group of heterogeneous materials based on their properties.

The system pilots study properties of powder materials although it can solve some practical problems, but they are in their development almost exhausted. So now is the development of analytical methods for studies that are able to detect and investigate more subtle physical and structural properties of powder materials.

At present promising methods properties of powder materials, which are based on mathematical modelling of structures. With them in the first place could be considered more subtle structural features that cannot capture the experimental methods; second, research is conducted with modern computer that allow large amounts of computation with high accuracy and in a short time; thirdly, the study of methods of mathematical modelling structure allows a very flexible and quickly carry out the necessary amendments and clarification of research methodology.

Problem.

The basis of any theoretical study is to create a mathematical model of the phenomenon, process steps. In our case, there is a need for a mathematical model of the structure of powder materials with which you can calculate and explore the physical and structural characteristics.

Mathematical modelling can solve problems for a wide class of powder materials. Many problems can be solved by representing the structure of powder materials simplest mathematical model. Mathematical modelling can be useful for substantiation of shapes and sizes of samples of powdered materials in experimental methods of study.

Mathematical modelling considered as a promising and multi-dimensional methods, using which it is possible decide important scientific, research and practical problem.

Main part.

With the advent of large core, high speed computers, as well as the new generation of low cost, mid-range minisystems, simulation approaches to real world problems are now reaching full bloom. Simulation software is now generally available for all levels of computer systems and configurations, and simulation societies and journals are now coming into being.

At creation mathematical model should be guided by the general principles of mathematical modelling. Firstly, the mathematical model abstracts from specific physical meaning and considers only the mathematical content of the physical phenomena that considers only the mathematical equation (or system), which can be described this physical phenomenon. Secondly, with all the mathematical description of physical phenomena selected only those equations and parameters that have a significant impact on the occurrence of this phenomenon. Bold are key aspects in the mathematical model allows, on the one hand, using a single mathematical model to investigate a number of similar phenomena and, on the other hand, analyse the impact of these or other side effects that appear in the basic model by introducing into the mathematical model of the amendments and refinements. These same principles can be applied to create a mathematical model of the structure of heterogeneous materials [1-5].

Having a specific task research a variety of physical and structural properties of the powder material, we can advance with reasonable certainty select the desired mathematical model. In the process of theoretical studies and comparing the results of experimental studies may clarify the mathematical model, which can be different for different character types of physical and structural properties. The main problem in the mathematical description of the structure of powder materials is its statistical nature.

With this in mind, we begin our discussion of a step-by-step approach to simulation modelling. In Fig.1, the step-by-step simulation modelling methodology is illustrated [6].

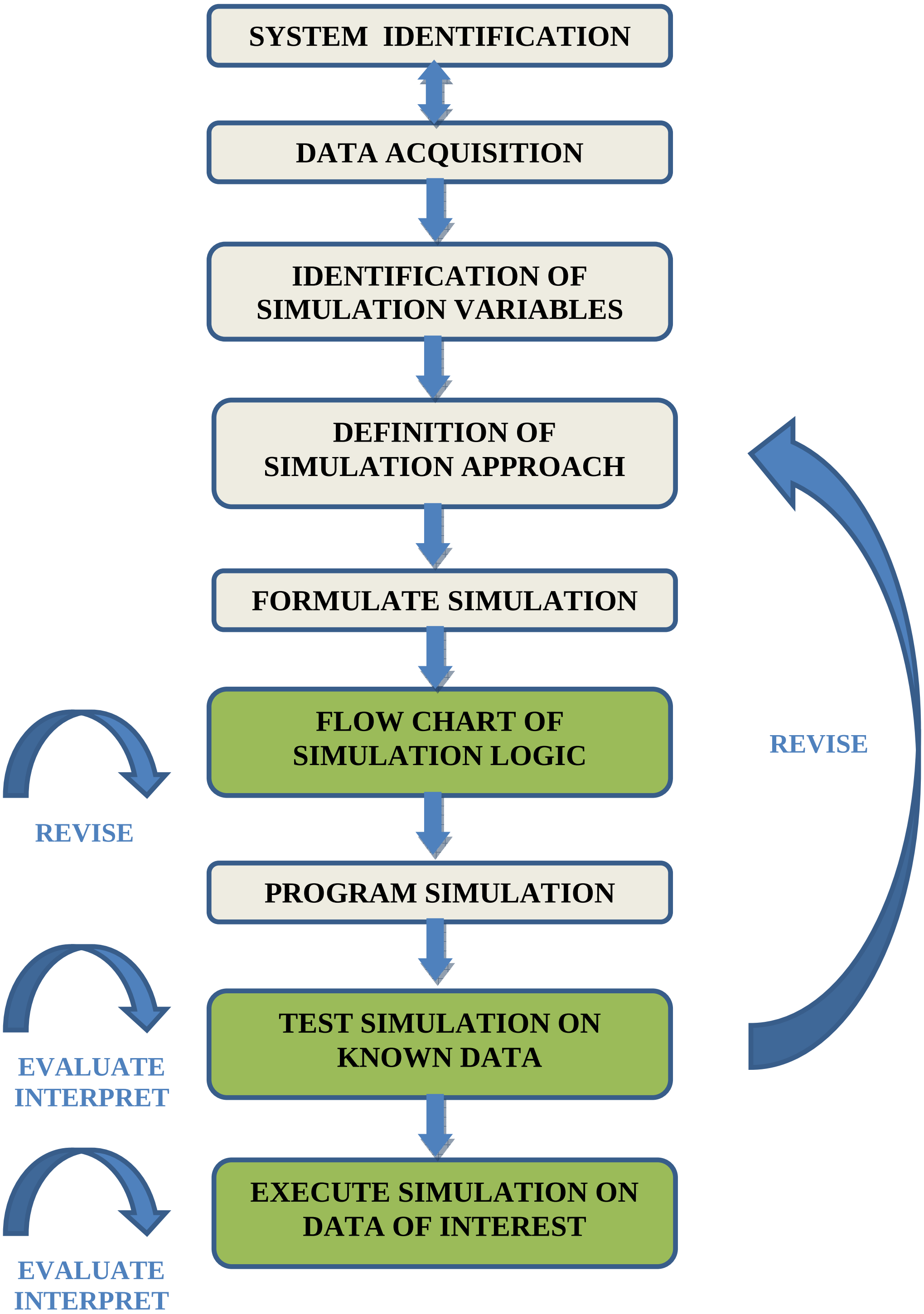

Fig.1. Step-by-step simulation modelling methodology

System identification.

As simple as it may appear to be, identification of the system to be simulated is a crucial step in the development of simulation. Questions of oversimplification or under simplification are of extreme importance, particularly when the results of the decision-making situation might be utilized in some type of medical therapy regimen or airport traffic planning program. One must remember that simulation involves the construction of some type of model which describes the system's operation in terms of individual events, elements, and/or components. Further refinements involve descriptions of the interrelationships between the components/elements of the simulation model. Thus, simulation is a means of dividing a model into its component parts and allowing one to investigate the results of the interactions between these parts.

Understanding how much or how little detail to place into a simulation model is one of the most difficult portions of the simulation scheme. It requires familiarity with the problem under investigation; i.e., what results are needed. It requires an understanding of the system to be simulated, hence the feedback between the data acquisition step and the system identification step in Fig. 1. Finally, it involves that elusive item known as "simulation experience." This comes only from having tried to formulate many simulations.

There is no real shortcut explanation which will tell a scientist how to plan a simulation which has just the right level of complexity. What we attempt to do, in our classes, is to illustrate cases involving too little or too much complexity for the output information required. Useful examples which can be made to display all levels of complexity may be found in such problems as inventory control, large harbour waiting time simulations, and airport control simulations. I have found that a canonical example of levels of simulation complexity may be found in modelling the behaviour of cellular systems [7, 8]. Depending upon what are the questions one wishes to answer, it is possible to build a very simple simulation model into one which is quite complex. If one illustrates the increase of complexity in the simulation as a function of the change in complexity/output information required by the question being put to the simulation model, then the scientists build up an association which allows them to see how a question requires a certain level of simulation complexity. Further, one may then take a complex simulation and show why, though it might answer a simple question, it was not necessary to go overboard when a less complex simulation would have sufficed.

Data acquisition.

Once the system for study has been identified, it is important to obtain as much knowledge/data on the system as is available. This is necessary for three important reasons:

- ✓ correct formulation of the simulation requires a well-balanced understanding of the real-world system and its behaviour. Data acquisition will help develop this understanding. This will hopefully lead to a realistic/"correct" formulation of the simulation logic;
- ✓ any simulation has parameters whose values must be somehow acquisition. Data acquisition usually yields actual values of the parameters. Or, in the case where it does not yield values, it often leads to insights as to how one might estimate the data values;
- ✓ when it comes time to test the accuracy of the simulation, data must be available to do so. An efficient data acquisition step usually.

Identification of simulation variables.

In this step we define our input, output, and "interstep" variables. The "interstep" variables are those variables whose calculation is necessary in order to get from the input variables to the output variables, as formulated from our system identification analysis.

Definition of simulation approach.

At this point, we are ready to define the form of the simulation. In general, our lectures tend to categorize the simulation types as follows: Simulation language-such as GPSS, DYNAMO, SIMPAC, GASP, or SIMSCRIPT; Analytic-this simulation approach makes use of analytic equations which describe the dynamical behaviour of the system - ABAQUS, MARC, Qform; Monte Carlo simulation; Mixed type-this simulation approach mixes some combination of the previous three types of simulation.

Formulate simulation model.

At this stage of our methodology, we begin the actual formulation of the simulation. This may be simply a block diagram showing a rough logic flow; or, it may be a diagram with the appropriate equations/rules annotated in the correct positions.

Flow chart simulation model.

While it is not always necessary to flowchart simulation logic, we emphasize the efficiency of this step; particularly to beginners in the simulation world. At this point we also have a brief discussion of flow chart semiology and logic. It is important to emphasize that this is the first step where logic errors, as well as inaccuracies in formulation and system identification, may occur and be corrected. This is why we have a revision loop at this step.

Program simulation model.

This step is self-explanatory. The are encouraged making use of CRT terminals, batch processing, or non-CRT terminal input methods to program their simulation. Programming may be done in any number of available programming languages or simulation languages.

Test simulation or known data.

The importance of this step cannot be overemphasized. We have found that the general attitude in simulation is one of “now that I’ve gotten the thing programmed and running, it must work correctly.” Hence, we emphasize this step as a second check in our simulation methodology. Here, we use available data on the real world system as a check on the behaviour of our simulation model. Excessive deviation between the two necessitates revaluation and revision of the simulation.

Evaluate simulation on data of interest.

At this. point, if all has gone well, and we have a reasonable level of confidence in our simulation model, then we are set to evaluate our simulation on the data of interest.

Conclusion.

According to this method can be calculated any structurally heterogeneous characteristics through specific programs that combine algorithms model the random filling of powder materials.

In the simulation modelling and prediction of the properties of powder materials can be considered the following tasks:

1. Microscopic study of the relationship of structural and physical properties of the compositions of the powder material structure.
2. Study of the formation of structures with desired geometric properties.
3. Research capabilities of process management structure formation in order to obtain materials with optimal properties required.

1. K. Sobolev, A. Amirjanov, Application of genetic algorithm for modeling of dense packing of concrete aggregates, Constr. Build. Mater. 24 (2010) P.1449–1455.
2. K. Kristiansen, A. Wouterse, A. Philipse, Simulation of random packing of binary sphere mixtures by mechanical contraction, Physica A 358 (2005) P.249–262.
3. J. Kergadallan, G. Puente, P. Doremus, and E. Pavier: Proc. Int. Workshop on "Modelling of metal powder forming processes", Grenoble, France, 2007, P.277-285.
4. M. Witten, Modelling cellular systems and aging processes: IV. Simulation of an asynchronously dividing cellular system, in Proc. Summer Simulation Symposium, PP.439-l43 (1981).

A. Darelius, A. Rasmuson, I.N. Bjorn, S. Folestad, High shear wet granulation modelling – mechanistic approach using population balances, Powder Technology 160 (3) (2005) P.209–218.

5. J. Spanier, Thoughts about the essentials of mathematical modelling // J. Spanier “Math. Modelling”. - №1, 2008 - P.98-108.
6. K. Gotoh, A random packing structure of equal spheres G statistical geometrical analysis of tetrahedral configurations, Powder Technol. 20 (2008) P.233–242.
7. R.M. German, S.J. Park, Mathematical Relations in Particulate Materials Processing: Ceramics, Powder Metals, Cermets, Carbides, Hard Materials, and Minerals, Wiley, 2008.