THE ROLE OF COMPUTER SIMULATION IN NUCLEAR TECHNOLOGIES DEVELOPMENT

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ABSTRACT

In the report the role and purposes of computer simulation in nuclear technologies development is discussed. The authors consider such applications of computer simulation as nuclear safety researches, optimization of technical and economic parameters of acting nuclear plant, planning and support of reactor experiments, research and design new devices and technologies, design and development of "simulators" for operating personnel training. Among marked applications the following aspects of computer simulation are discussed in the report: neutron-physical, thermal and hydrodynamics models, simulation of isotope structure change and damage dose accumulation for materials under irradiation, simulation of reactor control structures.

INTRODUCTION

The second half of the twentieth century will come into history as time of fast development of scientific technologies and their wide application practically in all parties of human activities.

One of the most important achievements of modern science is the appearance and wide application of computer simulation. The computer simulation is a powerful tool of scientific researches. It has opened up new fields of researches, has given new qualitative impetus for science and scientific technologies development. Employment of computer simulation has essentially increased the efficiency of scientific researches and made these researches faster and cheaper. Also it has expanded a sphere of objects under research.

In the report the role and purposes of computer simulation in nuclear technologies development is discussed. One of cardinal directions of application of the simulation, and this direction is especially characteristic of nuclear engineering, is nuclear safety researches. For such problems the computer simulation is especially suitable and sometimes the only method of their solution.

Also it is necessary to emphasize such applications of computer simulation as:

- optimization of technical and economic parameters of nuclear plant operation,
- planning and support of reactor experiments,
- research and design of new devices and technologies,
- design and development of "simulators" for operating personnel training.

Obviously, it is impossible to give the absolutely complete and detailed overview of all sections of computer simulation and its applications for nuclear technologies development in one report. Therefore only the most significant and actual aspects of this problem are considered in the report.

THE SCHEME OF COMPUTER MODEL CONSTRUCTING

Let there be required to construct a computer model of some physical object, phenomenon or process. Then the scheme of such constructing looks as it is shown in a Fig. 1 (Samarsky, 1984 and Samarsky, 1989). The fundamental laws that control the object of research are formulated and the corresponding *mathematical model* is constructed. Usually the mathematical model is a presentation of the laws in mathematical form (the system of algebraic, differential, integral, logic equations, et cetera). At a mathematical model constructing we neglect the factors which don't have important influence on the process under study.

After the problem is formulated in the mathematical form, it is necessary to start with developing an *algorithm* for its solution. Here algorithm is assumed as such interpretation of mathematical model that allows its realization with the computer.

For implementation of the designed algorithm it is necessary to compile and to debug the corresponding *computer code*. Further, for the composed and debugged computer code it is necessary to prepare *input data* describing a concrete state of the initial object, and *libraries* of requisite parameters (for example, libraries of physical constants or neutron-physical cross-sections).

The designed computer code with the prepared set of input data and libraries of parameters make up a *computer model* of the object under research.

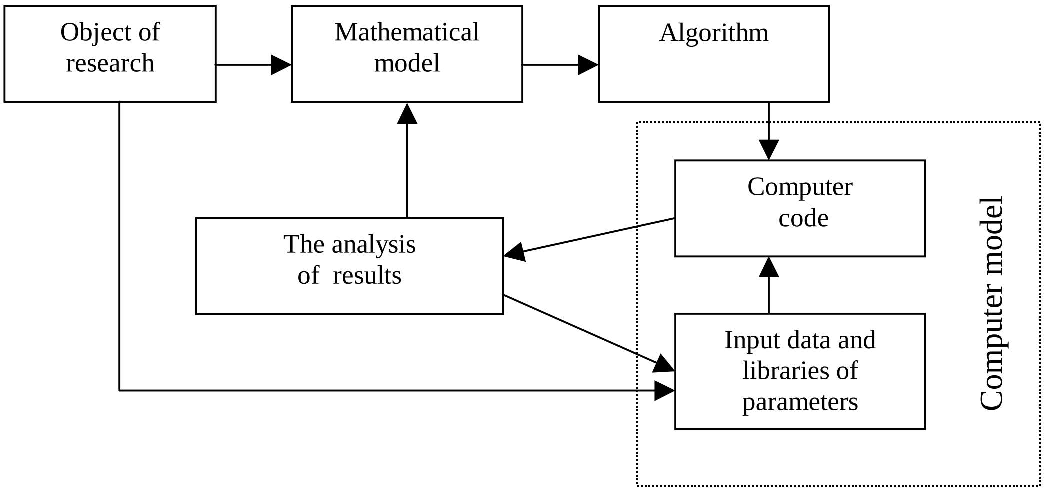

FIGURE 1. The scheme of computer model constructing

After completion of computer model constructing the stage of its verification follows. At this stage the results obtained from the model are analysed, and the adequacy of the constructed model to the object under research is estimated. If necessary the mathematical model and input data are refined, the scheme of algorithm is amended.

SECTIONS OF COMPUTER SIMULATION

Here we shall consider the main sections of computer simulation as applied to researches in the nuclear technologies area.

The neutron-physical and thermal-hydraulic models

The neutron-physical and thermal-hydraulic models have a very important role in investigations of properties and obtaining a broad spectrum of physical characteristics both for operating and designed nuclear-power plants, devices, fissile material storages etc. The long-term employment experience of the models has shown their high efficiency in the solution of different problems of nuclear engineering. They have found especially wide application where the acquisition of the qualitative experimental information is laborious or impossible.

The most significant use of the models is their broad application in works related to nuclear safety researches. Using these models the behaviour of plants in abnormal conditions and malfunction is investigated. The investigations allow to forecast consequences of these conditions, to estimate a probability and degree of possible negative effects and to take steps for their reduction.

The neutron-physical and thermal-hydraulic models are successfully applied for planning and computing support of reactor campaigns. They allow the optimum conditions for reactor experiment realization to be selected. It facilitates the improvement of technical and economic parameters for nuclear plants operation and allows an increase of the efficiency of researches.

The neutron-physical computer codes, which are a base for the models under consideration, can be arbitrarily divided into two classes: the class of precision codes and class of engineering codes.

The programs from the class of precision codes allow the most sensitive numerical algorithms to be implemented and computer models to be constructed with the detailed description of the objects geometry. Precision codes, where a method of analogue simulation of particles transfer is implemented – the Monte-Carlo method, showed a very good performance. For such programs, as a rule, the high precision of output results is characteristic ($\pm 0.3\%$ $\Delta K/K$ at calculations of criticality). However with all their advantages an essential disadvantage of such codes is their low-level computation rate. From the most known and popular precision codes it is necessary to draw attention to such computer codes as MCNP (Briesmeister, 1993), MCU (Gomin, 1995), KENO (SCALE, 1995). On the basis of a MCU computer code the neutron-physical models of research reactors SM-2, RBT-6 and MIR (Tsikanov, 1991) are designed and successfully operated in SSC RF RIAR.

The engineering codes have a higher computation rate than the precision codes. But they have a little less precision. The neutron-physical characteristics of nuclear-power plants may be operatively calculated by these codes. They also allow the effective planing and simulation of a reactor campaign. Now, such known engineering codes as TRIGEX (Seregin, 1985) and JAR (Yaroslavtseva, 1983) are successfully used at our institute for computing support of the fast reactor BOR-60 (Tsikanov, 1991) operation. By virtue of the high computation rate the engineering codes can be successfully applied in computer simulators intended for operating personnel training.

Among computer codes used for constructing of thermal-hydraulic models the most popular and conventional computer codes are such as RELAP5/MOD3 (Carlson, 1990) designed in INEL, and also RETRAN, CATHARE, TRAC, HTRF Data codes (Min Lee, 1990).

Simulation of damage of materials under irradiation

Radiation damage is one of the important characteristics of radiation effects. It used in research of changes in physical and mechanical properties of materials under long-term irradiation. In conditions of high neutron fluxes the materials undergo change of their properties. The changes are caused by transmutations and structural modifications at an atomic level. The reliable evaluation of radiation damage allows the comparison of different conditions of irradiation and the forecast of materials behaviour depending on a radiation effect dose in operating or designed reactors.

In studies of the property changes of the materials under irradiation and in defining their suitability for these or those units it is very important to obtain true information on the results of radiation effects, that is: damage dose. It is defined as the amount of displacements per atom (dpa), caused by neutron fluence.

Experts in the field of reactor materials technology and reactor dosimetry have agreed the procedure of damage dose calculations for the last 15 years. The procedure corresponds to the NRT-standard (Norgett, 1975). The procedure developed at ANL by Larry Greenwood in 1985 (Greenwood, 1985) is considered the most progressive and representative.

However in the last years new models of radiation damage have been developed. The models allow a more correct to evaluation of the damage effects for different energy groups of a neutron spectrum. When the cascades of displacements are developing one part of the produced defects annihilates and another part affiliate with immobile clusters. Therefore now many researchers are inclined to believe that the registration of freely migrating defects (FMD) (Wiedersich, 1991) fractions is needed in comparison of materials irradiation results at different spectra of bombarding particles.

The modern computer simulation of processes of materials structural changes is based on the molecular dynamics methods (Kirsanov, 1990). The molecular dynamics method is one of the main methods for analytical investigation of defect formation processes in solids. This method is based on solution of the Newtonian mechanics equations for a solid consisting of N atoms. When initial positions and velocity vectors of each atom are known, it is possible to simulate evolution of such a solid behaviour by a numerical solution of the system of 6N equations for velocities and coordinates of atoms. For the first time the molecular dynamics models in physics of radiation damages were applied by Vineyard and Gibson (Gibson, 1960).

The models based on the molecular dynamics methods are used for research of processes in cascades of displacements. The models allow to refine the damage constants to ring account of the fact that structure of a material changes under irradiation. In particular, the models are successfully used for refinement of the threshold displacement energy values for multicomponent materials and alloys (Markina, 1998 and Kirsanov, 1999).

Now one of the important problems of molecular dynamics simulation is the choice of a potential of interatomic interaction for different metals and alloys. Recently the atomic interaction potentials based on the "immersed" atom method are used more often (Daw, 1984 and Foiles, 1985). In this method the energy of each atom is calculated as energy necessary for immersing of an atom in electronic liquid formed from other atoms. In such a model the energy of the whole crystal is no longer the sum of couple interactions only. It is represented as a certain function of electronic density in a crystal and the interaction force of any two atoms is the function of local environment.

Simulation of reactor control structures

Constructing of a model of control structure, as well as designing of this structure, starts with the formulation of purposes of control and a system of criteria. They allow to judge the conformity of the system to these purpose (Glushkov, 1987). As a rule, such models have a module structure and discrete converters of the information describe the structure (Glushkov, 1987). In this case the automated control modules and those operated by people are differentiated. As a rule, such modules are described well by automata (final, determined, initial, probability etc.) (Kapmtonova, 1988). Now the simulation of such structures is widely applied for different areas of human activity for evaluating their efficiency and reliability.

In nuclear engineering an interest to the models has aroused foremost in connection with the development of computer simulators for improvement of professional skills and training of operation personnel.

It is necessary to emphasize that the simulation of control structures, in particular, allows the determined and probability evaluations of reliability and efficiency of such systems in case of malfunctions and personnel errors. Therefore in the near future one should expect their broad application for solving of problems of nuclear technology safety.

It is necessary to recognize that the application of these models for nuclear power engineering is not yet sufficient. Therefore, the task of development of such models is of great importance now. The simulation of reactor control structures should allow:

- optimization of these structures by different criteria,
- evaluation of their reliability,
- designing test systems to check their efficiency.

CONCLUSION

In the report the generalized scheme of computer models constructing is described. The role and purposes of computer simulation in development of the nuclear technologies is discussed. The authors showed the important role of computer simulation in solution of such problems as

- nuclear safety research,
- optimization of technical and economic parameters of nuclear plant operation,
- planning and support of reactor experiments,
- research and design of new devices and technologies,
- design and development of simulators for operating personnel training.

The brief review of computer simulation is given for such fields as

- neutron-physical and thermal-hydraulic models,
- simulation of isotope structure change and damage dose accumulation for materials under irradiation,
- simulation of reactor control structures.

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