MATHEMATICAL MODELS OF NUCLEAR ENERGY

Yu. A. Svistunov

Department of Applied Mathematics and Control Processes, State University of St-Petersburg, Russia

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Contents

Summary

This paper presents mathematical methods for modeling and optimization of processes which are used in nuclear power engineering. Introduction provides a brief description of how nuclear interactions are applied in various mankind activities. Consideration is given to arrangement of atomic nuclei, nuclear reactor and nuclear reactions which take place in reactor core and which are necessary for generation of heat energy. Modeling of these processes is considered as an example of nuclear installation modeling. It is impossible to design nuclear apparatus without optimizing their characteristics. One of the power optimization methods – Pontrjagin maximum principle is presented in this paper. The last section focuses on prospective nuclear-power engineering projects.

1. Introduction

Internal energy of atomic nucleus which is generated under nuclear transformations is nuclear energy. Nuclei consist of positive charged protons and electrically neutral neutrons. Protons and neutrons are commonly referred to as nucleons. Nucleons are attracted by nuclear forces and nucleons which have electrical charge are repulsed by

Coulomb forces. Energy which is spent for nucleus splitting is called bound energy E_b. Bound energy is determined by sum of attractive and repulsive energies of nucleons. This is the maximum energy which may be picked out.

Arrangement of nucleons and forces between particles inside nuclei determines the dependence of specific bound energy E_b/A on mass number A. E_b/A increases for light nuclei, decreases for heavy nuclei, and has the maximum value near mass number 56(*Fe*).

There are two kinds of exothermal nuclear reactions: a) fusion - formation of a light nucleus from lighter ones and b) fission - decay of a heavy nucleus. Because of Coulomb barrier, nuclear fusion reactions take place at high temperatures only. They are a source of stellar energy.

Attempts were made to produce nuclear fusion under earth conditions, but practical use of these results is still an open question. Only fission reactions are used now as a source of energy. For example, 0.86MeV/nucleon is actually picked out under ^{235}U nucleus fission reaction. Burning of 1g nuclear fuel in nuclear reactor provides 1MW*(twenty-four hours) of energy.

Therefore, nuclear power plants are main useful application of nuclear energy. Nuclear interactions, however, are extensively used in a variety of areas, such as medicine, investigation and change of material properties, customs control, etc. Thus, nuclear magnetic resonance is used as a diagnostic medical instrument. Many applications involve use of accelerators of charged particles - ions. Ions are formed from atoms which lose or join electrons.

Thus ions have electrical charge. Proton (nucleus of hydrogen atom) is the simplest ion. Many interesting examples of how accelerated ions can be used are ion implantation (changes in semiconductor properties), positron-emission tomography (universal medical diagnostic method), elemental analysis of material or environment, contraband detection system (in particular, detection of explosives and fission).

In last three cases, accelerated ions impinge special targets to produce neutrons or photons which go through research object and, in turn, produce secondary particles. Secondary particles (usually photons) carry information about object properties. This information is processed by the processing system.

Modeling of all these devices include modeling of particle dynamics and modeling of nuclear interactions in substance. These problems are embodied are presented in the mathematical model of nuclear reactor which is considered below. We may also mention some of the computer codes which are used for modeling physical processes in ion accelerators and reactor.

The best known are PARMILA and TRACE 3D - for modeling of particle dynamics, MAFIA - to calculate rf field distribution in resonators, set of codes ANSYS - for modeling of thermal processes.

2. Reactor Background.

Section of nuclear reactor is schematically shown in Figure.1.

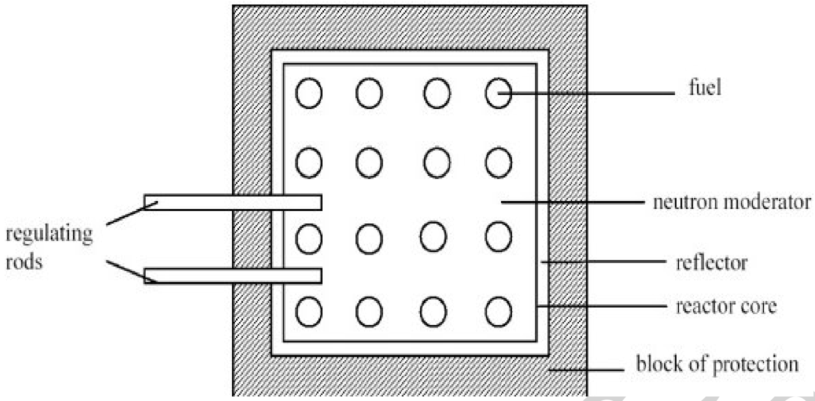

Figure.1 – Simplified scheme of reactor's section.

The main part of nuclear reactor is the reactor core, where nuclear fuel is placed. Chain reaction of fission takes in the reactor core and nuclear energy is picked out here. The reactor core normally has a cylindrical configuration. The quantity of fuel, which proves controlled chain reaction is called critical mass. When the reactor is loaded, nuclear fuel exceeds critical mass to compensate for fuel burning. Under normal operating conditions, nuclear fuel is regularly re-loaded. Nuclear fuel is placed inside fuel elements. There can be thousands and ten thousands elements. Coolant runs through the reactor core, comes into contact with fuel elements, and takes away the heat which is picked out from the elements. The heat then is transformed into electrical energy. The main processes, which take place in reactor core, are as follows: nuclear fission, radiative capture of neutrons, elastic and inelastic scattering of neutrons. Under fission, oncoming neutron is captured by nucleus, so that two radioactive fragments are formed and a few neutrons and gamma quantums are emitted. Quantity of secondary neutrons slightly increases with an increase in the energy of primary ones. The energy spectrum of fission neutrons ranges from 0 to 10MeV and is weakly-dependent on the energy of primary neutrons. After fission, some quantity of neutrons is emitted by exited nuclei which occur under β-decay of fragments. These neutrons are called delayed neutrons. An average ratio of the number of delayed neutrons to that of undelayed neutrons is close to one percentage. Probability of fission is determined by effective section of nucleus σ_f and strongly depends on the oncoming neutron energy. For low energies, this dependence at the average is *1/v* (where *v* is velocity of oncoming neutron). Here, some irregularities may also occur. They are determined by resonance capture of neutrons under low energies. Nuclei, which are formed under fission, have mass numbers ranging from 70 to 160 atomic units. They become stable after a few β-decays. 29% of fission fragments are gaseous *Kr* and *Xe*.

Section of resonance capture is denoted by σ_c. σ_c dependencies on energy are distinguished for both thermal neutrons and fast neutrons. With all energies of neutrons, elastic scattering holds for all nuclei. As a result, neutron loses part of its energy (if it is higher than heat energy) and gives it to recoil nucleus. Cross section of elastic scattering σ_s is weakly-dependant on energy. Post-scattering angular distribution of neutrons has isotropy. As a result, inelastic scattered neutrons lose a significant part of their energy, which goes to exile nuclei. Then it is irradiated as gamma-quantums. Part of energy passes to recoil nucleus. Section of inelastic scattering σ_{in} initially increases as energy exceeds the existing nucleus threshold and then passes to plateau. This constant is a geometric cross-section of nucleus. The parameters of chain reaction are determined by physical and geometrical properties of medium. After making relevant assumptions in respect of infinite medium, we may study these properties individually. Let K_∞ be a ratio of the number of present generation neutrons to the number of previous generation neutrons. Previous generation is represented by oncoming neutrons. Present generation is represented by secondary fission neutrons. Generation life time is very short $10^{-8}\ldots10^{-3}$sec, and hence neutron loss of β-decay (10^3sec) can be neglected. For homogeneous medium

$$K_\infty = \frac{\sum_i \vartheta_i \sigma_i \alpha_i}{\sum_i \left(\sigma_{fi} + \sigma_{ei}\right)\alpha_i}$$

where ϑ_i - number of fission neutrons, α_i - coefficients determining contributions of individual reactions. Finite medium has effective multiplication factor $K_{eff} < K_\infty$ because of neutron leakage form reactor core. When $K_{eff} = 1$, chain fission reaction is possible and this state is called critical.

3. Neutron Transport Equation

The behavior of nuclear reactor is determined by space, energy and heat distributions of neutrons. Therefore, the main problem of nuclear reactor theory is how to predict these distributions. Such distributions can be predicted by solving the neutron transport equation which is actually the Boltzmann equation of kinetic gas theory. The neutron distribution problem can be solved if we put into the transport equation the total set of interaction sections together with data of active reactor core accommodation. Then we may obtain numerical solution by employing Monte-Carlo method or some other method. In practice, however, it is impossible. First, energy-dependence of sections is very complex and sometimes they are unknown. Second, placing of materials in reactor is very complex too; thus, the transport equation may not be solved within reasonable time. Therefore, simplified forms of equation are usually used. Let us introduce some definitions and designations. In transport theory, neutron is considered as a pointed particle because de Broglie wave length of neutron is by an order of magnitude less than distance between atoms and by a few orders of magnitude less than average free length. Spin and magnetic moment have no significant effect on the neutron transport too. Further, neutron is taken to be a pointed particle. Its position and velocity are described by vectors $\vec{r}$ and $\vec{v}$, respectively. Velocity vector is usually presented as $\vec{v} = v\vec{\Omega}$, where $v = |\vec{v}|$ and $\vec{\Omega}$-vector which determines direction of motion ($|\vec{\Omega}| = 1$).

Neutron density is defined as $N(\vec{r},\vec{\Omega},E,t)$ (*E* is energy) and integral density is

$$n(\vec{r},E,t)=\int_{-1}^{1}\int_{0}^{2\pi}N(\vec{r},\vec{\Omega},E,t)d\varphi d\mu$$

$$\Omega_z=\cos\theta=\mu,\ \Omega_x=\sin\theta\cos\varphi,\ \Omega_x=\sin\theta\sin\varphi$$

in polar coordinate system. Product of velocity $\vec{v}$ and neutron density is called vector flux $\vec{v}N(\vec{r},\vec{\Omega},E,t)$

Absolute magnitude *vN* is neutron flux denoted as

$$\Phi(\vec{r},\vec{\Omega},E,t)=vN(\vec{r},\vec{\Omega},E,t),\ vn=\int\Phi(\vec{r},\vec{\Omega},E,t)d\Omega$$

is integral flux. If $\hat{n}$ - unit vector, perpendicular to surface, so that $\hat{n}dA$ is vector perpendicular to element of surface dA , then

$$\hat{n}dA\vec{v}N(\vec{r},\vec{\Omega},E,t)$$

number of neutrons crossing *dA* in unit solid angle over unit energy interval in unit time (if $\hat{n}dA\vec{v}<0$ crossing is negative). The total number of neutrons, crossing *dA*, is

$$\hat{n}dA\int_{4\pi}\vec{v}N(\vec{r},\vec{\Omega},E,t)d\vec{\Omega}$$

$$\int\vec{v}N(\vec{r},\vec{\Omega},E,t)d\vec{\Omega}=v\int_{4\pi}\vec{\Omega}N(\vec{r},\vec{\Omega},E,t)d\vec{\Omega}\equiv\vec{J}(\vec{r},E,t)$$

is called neutron current.

The basic form of neutron transport equation is

$$\frac{\partial N}{\partial t}+v\vec{\Omega}\cdot\nabla N+\sigma vN=\iint\sigma' fv'N'd\Omega'dE'+Q$$

The transport equation describes behavior of neutron group over time. σ'- total differential section for all types of interactions of neutrons with energy $E,\sigma' f$ – probability of transition from state $(E',\vec{\Omega}')$ to state $(E,\vec{\Omega})$ as a result of collision. $\partial N/\partial t$ is change of neutron density over time at point $\vec{r}$; $v\vec{\Omega}\cdot\nabla N$ - is change of neutron density as a result of neutron leakage; σvN - is velocity of neutron leakage as a result of collisions; first term of the right part (1) is change of neutron density as a result of influx of neutrons from other groups due to collisions; *Q* – is change of neutron density due to external sources. The transport equation may be written in terms of neutron flux $\Phi = vN$, ($\Phi' = v'N'$)

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} + \vec{\Omega}\cdot\nabla\Phi + \sigma\Phi = \iint \sigma' f \Phi' d\Omega' + Q$$

Solution of transport equation has often to be sought for in regions where surfaces separate two mediums which have different properties. The transport equation must be proved on both sides of the boundary. Therefore, the continuity condition must hold:

$$\lim_{s\to 0}[N(\vec{r}_s + 1/2\, s\vec{\Omega}, \vec{\Omega}, E, t + \frac{s}{2v}) - N(\vec{r}_s - 1/2\, s\vec{\Omega}, \vec{\Omega}, E, t - \frac{s}{2v})] = 0,$$

if the separation surface passes through point $\vec{r}_s$.

Boundary conditions on free surface in the absence of external sources must be

$$N(\vec{r}, \vec{\Omega}, E, t) = 0 \text{ if } \hat{n}\vec{\Omega} < 0.$$

4. General Properties of Transport Equation

The system including fission nuclei can be subcritical or above-critical. The system is subcritical when for any initial neutron generation $N > 0$ after long time will be passed, i.e. for $t \to \infty$, expected density $N = 0$ if there are no external neutron sources. The system is above-critical when expected density $N \to \infty$ as $t \to \infty$ for any small initial neutron generation. Finally, the system is critical when constant expected neutron density is supported in the system without external sources. The transport equation together with boundary conditions determines behavior of neutrons in the system being studied. If at $t = 0$ neutron density $N(\vec{r}, \vec{\Omega}, E, 0)$ is given, the expected density for any time can be determined by solving the transport equation. We have shown that such solution exists and is unique if sections and boundary conditions satisfy some mathematical conditions, which are practically always are met. We shall now consider criticality of system in terms of behavior of solution. Homogeneous (without sources) transport equation may be written as

$$-\frac{\partial N}{\partial t} = -v\vec{\Omega}\cdot\nabla N - \sigma v N + \iint \sigma' f v' N' d\vec{\Omega}' dE' = \hat{L}N$$

where $\hat{L}$ - operator. Let us consider the solution of equation

$$-\frac{\partial N}{\partial t} = \hat{L}N$$

as

$$N = N(\vec{r}, \vec{\Omega}, E)\exp(\alpha t)$$

Then

$$\alpha N(\vec{r},\vec{\Omega},E)=\hat{L}N(\vec{r},\vec{\Omega},E)$$

Many eigenvalues α_j exist and they have relevant eigenfunctions N_j - solutions of transport equations i.e. $\alpha_j N_j = LN_j$. Let us assume that solution can be presented as a series over eigenfunctions N_j. If α_0 is the value of α_j having maximal real part, then we may expect, when t is great, that solution will be proportional

$$N_0(\vec{r},\vec{\Omega},E)\exp(\alpha_0 t).$$

The difference between subcritical and above-critical systems is determined by the sign of eigenvalue α_0. Physically, we may assume that α_0 is real i.e. oscillations of neutron density are absent. Further, N_0 must be no negative, because negative values of neutron density are impossible. Then for subcritical system $\alpha_0 < 0$, for critical system $\alpha_0 = 0$, for above-critical system $\alpha_0 > 0$. That is, the problem of criticality reduces to the problem of sign α_0 determination.

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Biographical Sketch

Yuri A. Svistunov, is doctor of science, professor of Department of Applied Mathematics and Control Processes of St.Petersburg State University, Scientific Research Accelerator Laboratory Head of D.V. Efremov Institute (NIIEFA).He was born in 1938 in Leningrad (USSR). His childhood fell on Leningrad blockade and post-war years. On leaving school and secondary radio engineering school, he studied at the

University of Leningrad specializing on theoretical physics. From 1963 to present time he is scientific worker of D.V. Efremov Scientific Research Institute of Electrophysical Apparatus. Since 1989 he teaches in Leningrad (Saint Petersburg now) State University and later (1994) became a professor of University. His collaboration with Russian Academy Associate Member V.I. Zubov and Zubov's team of scientists resulted creation of control theory of accelerated charged particle beams. This theory is used broadly now on accelerator designing. His others works are devoted to forming and acceleration precise ion beams, creation of contraband detection systems and safe electronuclear installations. He lives in St.Petersburg.