THE NEUTRONS FLUX DENSITY CALCULATIONS BY MONTE CARLO CODE FOR THE DOUBLE HETEROGENEITY FUEL.

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ABSTRACT

This document provides the calculation technique for the fuel elements which consists of the one substance as a matrix and the other substance as the corns embedded in it. This technique can be used in the neutron flux density calculation by the universal Monte Carlo code. The estimation of accuracy is presented too.

Introduction

The materials of the irregular composition came into use in the reactor technology recently. Such material is comprised of two substances. The second substance forms spherical corns the size of the order of 0.5 mm, which are positioned in the media of the first substance. The total volume of the corns account for 1% of the total volume of the material. The location of the corns in the first substance designated as a matrix is casual enough.

An important point is that the following two conditions are fulfilled for the existed energy regions.

- The macroscopic cross sections of the corns is more than one of the matrix by a factor of 10.
- The product of the macroscopic cross section of the corn into its diameter compares with 1.

In that case replacing the matrix and the corns with the homogeneous media during the calculations cannot be tolerated. The reasons are the same as for the intolerable homogenization of

the heterogeneous reactor [1].

Such materials are used for the production of the fuel elements. The fuel elements form the heterogeneous structure in the reactor. So they are referred to as being the double heterogeneity.

The fuel elements of this kind find use in the high temperature reactors [2]. It is often advisable to consider its application in thermal reactors [3].

Calculation technique

The standard technique of the neutrons flux density calculations by Monte Carlo code gives two opportunity. The first opportunity is the homogenization of the fuel material. This way is often impossible. The second opportunity is the consideration of each corn as the separate geometrical zone. This way is impossible because of a great number of corns. About 10^4 corns are contained in one spherical fuel element of the high temperature reactor.

So the special calculation technique for such systems has been developed on the base of the MCU code [4]. For its description we insert the following designations: The corns are equal in size and their radius is symbolized by r. The letter n denotes a number of the corns per unit volume. For the sake of simplicity assume that one fuel element is considered. The heterogeneous part of the fuel element is designated as region Q. Its volume is indicated by the symbol V_Q. The total number of the corns denoted by N is equal to $n*V_Q$. So the total volume of the corns denoted by V_K is equal to $4/3*\pi*r^3N$, and the volume of the matrix denoted by V_M is equal to V_Q-V_K.

Let us denote a set of the positions of all corn centres by B_M. We assume that two or more corns can be located in the same part of the space. That proposal gives that B_M is equal to the Cartesian product QxQx...xQ which is taken N times. B_H will denote the set of the real positions of the corn centres in view of impossibility of the corns intersections. Random location of the corns implies that the function of the probability density on a set B_H is equal to the constant.

Obviously $B_H \subset B_M$, and if $V_f/V_M \ll 1$ then the differ $B_M \setminus B_H$ is small. In this case a set B_M can replace a set B_H during calculations. It means that the probability for neutron to enter a corn on the interval (s,ds) is equal to Sds, where $S=\pi r^2 n$. It is similar to the rule of the generation a macroscopic cross sections from microscopic ones. We use an algorithm derived from these presumptions. For the first time the similar technique was presented in [5].

Two frames of reference will be entered into consideration. The first frame of reference is used for the fuel element as a whole and the second one is used for a corn. For the motion in the first system the matrix with the corns is taken as the homogeneous media with the macroscopic cross section Σ_m equal to $\Sigma_{mt}+S$, where Σ_{mt} denotes the total macroscopic cross section of the matrix material. So, Σ_{mt}/Σ_m is the probability of the modeling of the interaction with the matrix nucleus. S/Σ_m is the probability of the modeling of the entrance into the corn.

After the entrance into the corn the frame of reference is changed. Clearly the point of the entrance is uniformly distributed on the projection of the corn on the plane which is perpendicular to the neutron velocity. The modeling of this point is simple enough. The location of the corn centre is uniquely determined by the point of entrance into the corn and the coordinates of that point with respect to the first frame of reference.

The modeling of the neutron trajectory in the corn follows the standard technique of the Monte Carlo calculations. In all carried out calculations the corn has been treated as the homogeneous sphere. However, that is not a particular problem to consider any type of the corns with spherical symmetry, for example, the sphere with the central part and a sheath. frame of reference If the scattering takes place in the corn then the coordinates of the corn centre and the coordinates of the collision point in the corn have been retained after the conversion of the energy and the velocity direction of the particle. After the neutron leaving of the corn the frame of reference is changed to the first one and the particle returns to the homogeneous media.

The algorithm is similar for the cases of the neutron absorption and the neutron generation as the result of the disintegration. If there is no collisions in the corn a great number of the parameters is retained. The last case stands out for the computational speed increase.

If the ratio V_K/V_M is not small enough, then it may be beneficial to correct the value S in the algorithm. Let the fuel element be intersected by the occasional straight line. Calling the expected value of the sum of the line segments in the matrix substance L_M and the expected value of the sum of the line segments in the corn substance L_K, the ratio V_K/V_M is equal to L_K/L_M. On the other side we have S entrances in the corns per unit straight line in this algorithm. So, calling the average chord d, the ratio $V_K/V_M=L_K/L_M=Sd$. Clearly $d=(4/3\pi r^3)/(\pi r^2)$, so $S=\pi r^2 n*V_Q/V_M$. The ratio V_Q/V_M is the difference from the given above expression.

Estimation of accuracy

The simple technique gives us the opportunity to estimate an error introduced by assuming that two or more corns can be located in the same part of the space. Calling the point of the neutron outlet of the first corn A, the neutron path before its entrance in the next corn at the point B is equal to s. The neutron moves at angle β with respect to the normal. The cross section of the entrance into the second corn at the point B is equal to S in our model. The centre of the second corn could be located at the upper half of the sphere with the centre at the point B and with the radius r. The value S/n is equal to the area of the projection of that half-sphere on a plane normal to the neutron path. (See Fig.)

To account for the impossibility of the corn intersections, the centre of the second corn cannot be located inside the sphere with radius 2r and the centre at the same point as the first corn has. So the part of the half-sphere that is inside that large sphere has to be removed. The real cross section labelled S_H is obtained from the projection of that remainder. The value S_H is the function of β and s parameters. $D(\beta)$ is a value such that if

$s<D$ then $S_H<S$, and if $s\geq D$ then $S_H=S$. The formulae for the functions $D(\beta)$ and $S_H(\beta,s)$ are derived with the use of the rudimentary knowledge of stereometry, but they are cumbersome.

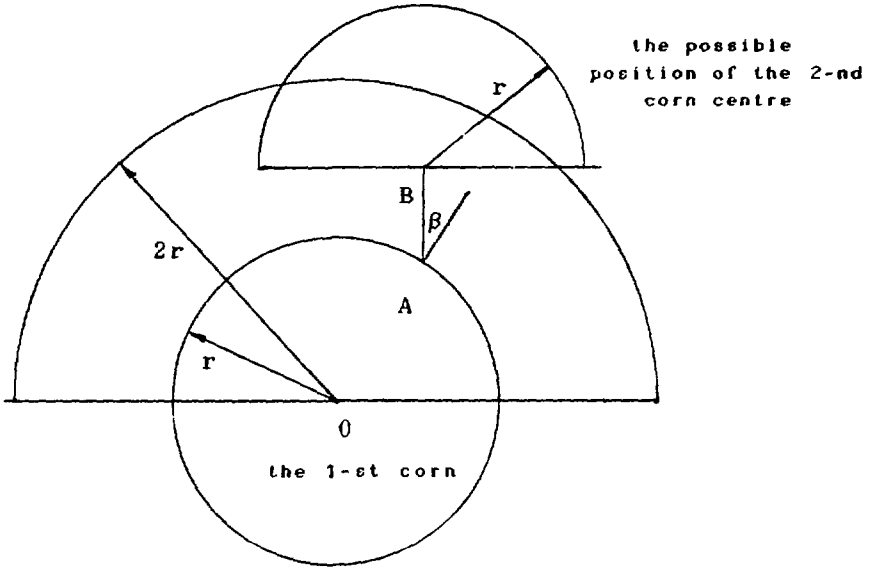

Fig. The corrections of the cross section of the corn entrance.

Using the approximation for small δ: $1-\exp(-\delta)=\delta$ and comparing S_H and S, we receive the following expression for the additional probability of the entrance into the corn:

$$P(\beta)=\int_0^{D(\beta)}(S-S_H(\beta,s))ds.$$

The total error of the model can be estimated as the average value of $P(\beta)$. It is reasonable to suggest that the distribution of β is appropriate to the isotropic flux. Hence the total error is the following:

$$\int_0^{\pi/2}\sin(2\beta)P(\beta)d\beta.$$

The model may be improved by using the technique of E.R.Woodcock [6]. Let us determine the function $g(\beta,s)$ as $S_H(\beta,s)/S$. Obviously $g(\beta,s)=1$ if the value s is large enough. The effective macroscopic cross section of entering into any corn, while the distance from the last leaving the corn is large

enough, is designated by the letter S_{ef}. The obtained at the last leaving angle β is put into the memory. If the neutron has not been in any corn since the last collision, the angle β is determined as -1. We suppose that $g(-1,s)=1$. The motion in the region Q is considered as the motion in the homogeneous media with the macroscopic cross section $\Sigma_m=\Sigma_{mt}+S_{ef}$ in a similar way to the first model. The ratio Σ_{mt}/Σ_m is the probability of the collision in the matrix substance, the ratio $S_{ef}g(\beta,s)/\Sigma_m$ is the probability of the entrance into the next corn, the ratio $S_{ef}(1-g(\beta,s))/\Sigma_m$ is the probability to continue in free motion.

The value S_{ef} must satisfy the following equation:

$$S_{ef}\int_0^{\pi/2}\sin(2\beta)\int_0^{\infty}sg(\beta,s)\exp(-S_{ef}\int_0^{s}g(\beta,\sigma)d\sigma)dsd\beta=4rV_M/V_K$$

The left side of this equation is the expected value of the part of the trajectory between two corns under the condition that $\Sigma_{mt}=0$.

That refining technique has not been included into MCU code yet.

Example

By way of example let us consider a calculation of the infinite lattice of the spherical fuel elements. The centres of the fuel elements form the diamond lattice. The fuel elements are situated in the free space, each element consists of the graphite sheath with heterogeneous sphere inside it. The heterogeneous material consists of the graphite matrix and the corns made from the uranium oxide. The total radius of the fuel element is equal to 6 sm, the radius of the heterogeneous part is equal to 5 sm, the diameter of the corn r is 0.0502 sm, the total number of the corns in the one fuel elements is 9400.

The calculation by double heterogeneous technique gives $k_{ef}=1.697$. After the homogenization of the corns in the inside part of the fuel element the standard calculation technique gives $k_{ef}=1.590$. So a gap between these two techniques achieves 6.6%.

On the other side the total error estimated as given above is equal to $2.7*10^{-3}$. There is the satisfactory result.

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