

# Numerical Calculation of Neutron Kinetics for Multiregion and Two Energy Groups

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2군에너지 및 혼합 매질에서의 중성자 동특성의 수치해석

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## 1. Introduction

A computer program written in Fortran is developed for the calculation of prompt reactor transients. The underlying equations utilized in the Program are of nonlinear coupled space time kinetic equations. Two neutron energy groups are allowed with one spatial dimension and the reactivity feedback is incorporated. Since time and space are not separated (Duderstadt, J. J., 1976), it can describe a continuous spatial and time behavior of the flux. Particular attention has been given to the reduction of the numerical truncation error as well as to the minimization of the computation time, which are contradictory each other in general. To optimize these two factors of error reduction and computation time, timestep size has been made to change automatically as far as the magnitude of error during the computation process is tolerable.

## 2. Theory

The general two group one dimensional equations with delayed neutrons are (RETRAN-02, 1981):

$$\begin{aligned} \text{Group 1: } & \frac{1}{v_1(x,t)} \cdot \frac{\partial \phi_1(x,t)}{\partial t} = \nabla \cdot D_1(x,t) \nabla \phi_1(x,t) \\ & - [\Sigma_{a1}(x,t) + \Sigma_{12}(x,t)] \phi_1(x,t) \\ & + (1 - \beta) \left[ \sum_{i=1}^2 \nu \Sigma_f^i(x,t) \phi^i(x,t) \right] \\ & + \sum_{i=1}^{ND} \lambda_i C_i(x,t) \\ \text{Group 2: } & \frac{1}{v_2(x,t)} \cdot \frac{\partial \phi_2(x,t)}{\partial t} = \nabla \cdot D_2(x,t) \nabla \phi_2(x,t) \\ & - \Sigma_{a2}(x,t) \phi_2(x,t) + \Sigma_{12}(x,t) \phi_1(x,t) \\ \text{Delayed precursor: } & \frac{\partial C_i(x,t)}{\partial t} = \beta_i \left[ \sum_{i=1}^2 \nu \Sigma_f^i(x,t) \phi^i(x,t) \right] \\ & - \lambda_i C_i(x,t) \dots\dots\dots (1) \end{aligned}$$

where  $\beta = \sum \beta_i$ , and ND=number of delayed neutron groups.

All cross sections used in the above equations are energy averaged values and are functions of position and time to describe absorbing rod movements and neutron energy changes. In Eq. (1), the time and space derivations are normally approximated as (Kuo. S., 1972)

$$\frac{\partial \phi(x,t)}{\partial t} = \frac{\phi(i,t+1) - \phi(i,t)}{\Delta t}, \quad \frac{\partial^2 \phi(x,t)}{\partial x^2} = \frac{\phi(i+1,t) - 2\phi(i,t) + \phi(i-1,t)}{\Delta x^2}$$

where  $i$  refers to  $i$ -th spatial mesh points and  $t$  refers to  $t$ -th timestep. However in using eq. (1), the following relation between the space and timestep interval should hold to ensure the decay of any induced errors (Young. D. M., 1972).

$$\Delta t < \frac{\Delta x^2}{2Dv} \dots\dots\dots (2)$$

where  $D$  refers to diffusion coefficient and  $v$  to neutron velocity. It is evident, from above equation, that if a normal finite difference method is used, very short timesteps should be employed to ensure the error decay, which results in a long computation time.

The theoretical equations can be modified into the numerical form as below. All the physical characteristics are assumed to be constant over the specific nodal volume and the values are averaged ones evaluated at the mid point of the mesh.

Let  $V(i)$ =volume of  $i$ -th region

$S(i)$ =surface area between regions  $i-1$  and  $i$

$J(i, j, t)$ =net current from region  $i-1$  to  $i$  for  $j$ -th energy group at time  $t$   
( $j=1$  for fast and  $j=2$  for thermal).

Then the balance equations of the  $i$ -th nodal volume can be established by introducing

$\frac{1}{v(i,j,t)} \frac{\partial \phi(i,j,t)}{\partial t}$  = rate of change of neutron density per unit volume

$\sum_a(i,j,t)\phi(i,j,t)$ = absorption rate per unit volume

$\nu \sum_f(i,j,t)\phi(i,j,t)$  = fission rate per unit volume

$\sum(i, j \rightarrow j-1, t)\phi(i,j,t)$  = slowing down rate per unit volume

$\sum_{n=1}^{ND} \lambda_n C(i,n,t)$ = delayed neutron source per unit volume

$[J(i,j,t)S(i) - J(i+1,j,t)S(i+1)]/V(i)$ =net leakage from region  $i$  per unit volume =Leakage.

In addition, the neutron current density  $J(i, j, t)$  can be obtained by imposing the boundary conditions. That is, by defining the  $\phi'(i, j, t)$  be the flux at the interface between  $i-1$ th and  $i$ th nodal volume. Then,

$$\frac{-D(i-1,j,t) \cdot [\phi'(i,j,t) - \phi(i-1,j,t)]}{\Delta x(i-1)/2} = \frac{-D(i,j,t) [\phi(i,j,t) - \phi'(i,j,t)]}{\Delta x(i)/2} \dots (3)$$

Rearranging,

$$\phi'(i,j,t) = [\phi(i-1,j,t) + \frac{D(i,j,t)\Delta x(i-1)\phi(i,j,t)}{D(i-1,j,t)\Delta x(i)}] \sqrt{[1 + \frac{D(i,j,t)\Delta x(i-1)}{D(i-1,j,t)\Delta x(i)}]} \dots\dots\dots (4)$$

Plugging this into current equation yields

$$J(i,j,t) = \frac{-2D(i-1,j,t)D(i,j,t)[\phi(i,j,t) - \phi(i-1,j,t)]}{D(i-1,j,t)\Delta x(i) + D(i,j,t)\Delta x(i-1)} \dots\dots\dots (5)$$

By the use of the relations defined above, the analytical balance equations for the  $i$ -th node are expressed in numerical equations of:

$$\begin{aligned} \frac{1}{v(i,1,t)} \frac{\partial \phi(i,1,t)}{\partial t} &= \text{Leakage}(i,1,t) \\ &- [\Sigma_a(i,1,t) + \Sigma_R(i,1,t)] \cdot \phi(i,1,t) \\ &+ (1-\beta) \left[ \sum_{j=1}^2 \nu \Sigma_f(i,j,t) \cdot \phi(i,j,t) \right] \\ &+ \sum_{n=1}^{ND} \lambda_n C(i,n,t), \end{aligned}$$

for fast group ..... (6)

$$\begin{aligned} \frac{1}{v(i,2,t)} \frac{\partial \phi(i,2,t)}{\partial t} &= \text{Leakage}(i,2,t) \\ &- \Sigma_a(i,2,t) \cdot \phi(i,2,t) \\ &+ \Sigma_R(i,1,t) \cdot \phi(i,1,t) \end{aligned}$$

for thermal group ..... (7)

$$\begin{aligned} \frac{\partial C(i,n,t)}{\partial t} &= \beta_n \sum_{j=1}^2 \nu \Sigma_f(i,j,t) \cdot \phi(i,j,t) \\ &- \lambda_n C(i,n,t), \end{aligned}$$

for delayed neutrons ..... (8)

These equations are employed in numerical calculations with the boundary conditions of zero flux and zero current at the boundary and with the conditions of symmetry.

In Eqs. (6) and (7), the right hand sides are comprised of leakage term, source term and sink term.

Again let  $S(i,1,t) = (1-\beta) [\sum \nu \Sigma_f(i,j,t) \cdot \phi(i,j,t)] + \sum \lambda_n C(i,n,t)$  and  $S(i,2,t) = \Sigma_R(i,1,t) \cdot \phi(i,1,t)$ .

Then equations (6) and (7) can be expressed in the form of:

$$\begin{aligned} \frac{d\phi(i,j,t)}{dt} &= v(i,j,t) \left[ \frac{\text{Leakage}(i,j,t)}{\phi(i,j,t)} \right. \\ &\left. + \frac{\text{Source}(i,j,t)}{\phi(i,j,t)} \right] - v(i,j,t) \text{Sink}(i,j,t) \end{aligned}$$

..... (9)

The sink term for group 1 is  $\Sigma_a(i,1,t) + \Sigma_R(i,1,t)$  and  $\Sigma_a(i,2,t)$  for group 2.

Therefore by defining

$$\begin{aligned} v(i,j,t) \left[ \frac{\text{Leakage}(i,j,t)}{\phi(i,j,t)} + \frac{\text{Source}}{\phi(i,j,t)} \right. \\ \left. - \text{Sink}(i,j,t) \right] &\equiv A(i,j,t) \end{aligned}$$

..... (10)

Eq. (9) is simply in the form of

$$\frac{d\phi(i,j,t)}{dt} = A(i,j,t) \cdot \phi(i,j,t) \text{ ..... (11)}$$

If  $A(i,j,t)$  is known exactly the linear equation (10) can be integrated by direct numerical procedures to find out the flux at any time  $t$ . That is,

$$\phi(i,j,t) = \phi(i,j,0) \exp \left[ \int_0^t A(i,j,t') dt' \right]$$

.....(12)

With the proper initial value of  $A$ , new flux can be obtained and by the use of this new flux,  $A(t)$  of next step is obtained to calculate the next timestep flux, so on. Further let timesteps be  $t_{n-2}, t_{n-1}, t_n, t_{n+1}, \dots$ , and also let  $T_1(i,j) = [A(i,j,t_n) + A(i,j,t_{n-2})]/2$  and  $T_2(i,j) = [A(i,j,t_{n-1}) + A(i,j,t_{n-2})]/2$ . Then by extrapolation,

$$\frac{dA}{dt} = \frac{2(T_1 - T_2)}{t_n - t_{n-2}}$$

and new values of  $A$  is estimated as

$$A(i,j,t) \text{ estimated} = T_1(i,j) + \frac{dA(i,j)}{dt} \cdot t$$

..... (13)

This estimated value of  $A$  is checked against the calculated value obtained from Eq. (10), and the results are utilized to control the error truncation, which in turn is reflected on the selection of timestep interval.

### 3. Error Treatment

In Eqs. (10) and (11),  $A(i,j,t)$  and  $\phi(i,j,t)$  are coupled each other. In other words,  $A(i,j,t)$ , the 'constant' term of linear equation (11), is determined by the flux, which can lead to the error accumulation unless proper error truncation or error decay is made. From Eq. (10), by neglecting the source and sink terms,  $A(i,j,t)$  of convective term only is:

$$A(i, j, t) = \frac{v(i, j, t)}{\Delta x^2} \frac{D(i, j, t)}{\phi(i, j, t)} [\phi(i+1, j, t) + \phi(i-1, j, t) - 2\phi(i, j, t)] \dots\dots(14)$$

With the assumption that flux and  $A(i, j, t)$  can be written as the sum of real value and error,  $\phi$  and  $A$  are expressed as

$$\begin{aligned} \phi(i, j, t) &= \phi_0(i, j, t) + \delta \phi(i, j, t) \\ A(i, j, t) &= A_0(i, j, t) + \delta A(i, j, t) \\ \dots\dots\dots(15) \end{aligned}$$

From Eqs. (14) and (15), the error part of  $A(i,j,t)$  is

$$\begin{aligned} \delta A(i, j, t) &= (vD/\Delta x^2) \\ &\times \frac{[\phi(i+1, j, t) + \delta\phi(i-1, j, t) - 2\delta\phi(i, j, t)]}{\phi(i, j, t)} \\ &+ \frac{A_0(i, j, t) \delta\phi(i, j, t)}{\phi_0(i, j, t)} \dots\dots\dots (16) \end{aligned}$$

If only the error of  $i$ -th node is considered,

$$\begin{aligned} \delta A(i, j, t) &= \frac{-2vD}{\Delta x^2} \cdot \frac{\delta\phi(i, j, t)}{\phi(i, j, t)} \\ &+ A_0(i, j, t) \frac{\delta\phi(i, j, t)}{\phi_0(i, j, t)} \dots\dots\dots (17) \end{aligned}$$

Typical values of  $\Delta x=1\text{cm}$ ,  $v=10^6\text{cm/sec}$ ,  $D=1\text{cm}$ , with neglecting the second term yields  $\delta A(i,j,t)=2 \times 10^6 \delta \phi(i,j,t) / \phi(i,j,t)$ . This shows that even a very small error in flux induces tremendous errors of  $A(i,j,t)$ , which makes the

numerical procedure unstable. For a given time interval  $A(i,j,t)$  is estimated by extrapolation method of Eq. (13) and is compared with the calculated value of Eq. (10). If the error is small enough to be tolerated, timestep interval is increased by the amount of preassigned value. On the other hand, if the error is detected, the timestep interval is replaced by the value which satisfies the normal finite difference equation. Since the timestep interval of this case results in stable process, the solution can continue with that value.

From Eq. (15),  $A(i,j,t)=A_0(i,j,t)+\Delta A(i,j,t)$ , and from Eq. (12).

$$\begin{aligned} &\frac{\phi(i, j, t + \Delta t)}{\phi(i, j, t)} \\ &= \exp \left[ \int_t^{t+\Delta t} A_0(i, j, t') dt' \right] \cdot \exp(\Delta A \cdot \Delta t) \\ &= \exp \left[ \int_t^{t+\Delta t} A_0(i, j, t') dt' \right] \cdot (1 + \Delta A \cdot \Delta t) \\ \dots\dots\dots (18) \end{aligned}$$

Rearranging with the separation of flux into correct and error terms,

$$\begin{aligned} \phi(i, j, t + \Delta t) &= \phi_0(i, j, t + \Delta t) \\ &+ \delta \phi(i, j, t + \Delta t) \\ &= \phi(i, j, t) \exp \left[ \int_t^{t+\Delta t} A_0(i, j, t') dt' \right] (1 + \Delta A \cdot \Delta t) \\ &= \phi_0(i, j, t + \Delta t) (1 + \Delta A \cdot \Delta t) \dots\dots\dots (19) \end{aligned}$$

therefore,  $\frac{\delta \phi(i, j, t + \Delta t)}{\phi(i, j, t + \Delta t)} \cong \Delta A \cdot \Delta t \dots\dots\dots(20)$

This shows that timestep interval can be controlled with the desirable flux error limits and with  $\Delta A$  obtained from the difference between the calculated and estimated values. With the determination of the flux over a given timestep interval, the delayed neutrons can be integrated

directly.

From Eq. (8),  $[d/dt + \lambda_n] \cdot C(i, j, t) = \beta_n \sum_f \nu \Sigma_f(i, j, t) \phi(i, j, t)$ . By introducing an integration factor,

$$\frac{d}{dt} [C(i, n, t) \cdot e^{\lambda_n t}] = \beta_n \sum_f \nu \Sigma_f(i, j, t) \cdot \phi(i, j, t) \cdot e^{\lambda_n t} \dots \dots \quad (21)$$

Again from Eq. (12).

$$\begin{aligned} &\phi(i, j, t) \\ &= \phi(i, j, t_0) \exp \left[ \int_{t_0}^t A(i, j, t') dt' \right] \\ &= \phi(i, j, t_0) \exp \left[ \frac{\int_{t_0}^t A(i, j, t') dt'}{\int_{t_0}^t dt'} \cdot (t - t_0) \right] \\ &= \phi(i, j, t_0) \exp [\bar{A}(i, j) \cdot (t - t_0)] \dots \quad (22) \end{aligned}$$

Then the result of the integration of Eq. (21) is.

$$\begin{aligned} C(i, n, t) &= \{ C(i, n, t_0) \\ &+ \beta(n) \sum_{j=1}^2 [\nu \Sigma_f(i, j, t_0) \cdot \phi(i, j, t_0) \cdot EXP] \} \\ &\times \exp [-\lambda_n (t - t_0)] \\ \text{where } EXP &= \frac{\exp \{ [\bar{A}(i, j) + \lambda_n] (t - t_0) \}}{\bar{A}(i, j) + \lambda_n} \\ &\dots \dots \dots \quad (23) \end{aligned}$$

All cross sections are assumed to be constant during the given interval.

#### 4. Results of Calculation and Discussion

A computer program in Fortran has been made based on the theory discussed above. As input to the program the data of TRIGA reactor is used.

The briefs are: 11 regions (5 regions in fuel and 6 regions in reflector), two energy groups (fast plus thermal) and cylindrical geometry. Initial system temperature is room temperature and the initial power is 1000 watt. Temperature feed-

back coefficients are considered. One delayed neutron group is modeled with  $\beta = 0.0079$  and  $\lambda = -0.08$  sec. with initial reactivity of 184 cents, the prompt transient are calculated up to  $t = 0.1$  sec. First, the computation speed is checked and summarized as below.

time interval, sec	number of calculations	maximum flux error
0.00 - 0.01	70	0.19326
0.01 - 0.02	40	0.19546
0.02 - 0.03	21	0.19717
0.03 - 0.04	12	0.19817
0.04 - 0.05	5	0.19932
0.05 - 0.06	5	0.19939
0.06 - 0.07	5	0.19936
0.07 - 0.08	5	0.19930
0.08 - 0.09	15	0.19932
0.09 - 0.10	89	0.00925

The above shows that up to 0.1 sec. total number of calculations is 257. However, during the time interval of 0.00 to 0.01 sec. since the system is unstable, a large number of computation is made in the program, which can be compared with the time interval of 0.04 thru 0.08 sec.

The number of calculation increases again during the final 0.90-0.10 sec, and with the aid of Figure 3, this can be interpreted that the system becomes unstable due to the effect of temperature defect.

The group 2 flux(thermal) is plotted against the distance from center in terms of time variation and extrapolation distances are neglected. Figure 1 shows that the thermal flux increases by about two decades during  $t = 0$  to  $t = 0.05$  sec and two decades during 0.05 to 1.0 sec. And in the reflector region the thermal flux increases slightly as well discussed in other literature(Lamarsh, J. R., 1966). Being compared with this is the fast flux.

in Figure 2, which increases by 3 decades during the first 0.05 sec, and about two decades during the last 0.05 sec, totaling 5 decades in 0.1 sec.

Figure 3 shows the change in power increase, center temperature against time and reactivity changes as well. As seen from the figure, the power(flux) increases exponentially, but the temperature response is almost constant up to 0.06 sec and then increases to about 38 C at  $t=0.1$  sec. This delay in temperature response is due to the system conductivity, of course. And the reactivity, which shows an abrupt increase due to initial positive coefficients, goes on with the

constant value of about 190 cents and drops as the temperature increases, which tells the effect of temperature defect.

The calculation system is not of separated position and time, hence can be used to check the limitation of the point model together with actual experimental data. Also as can be seen from Figure 3, the system is still unstable during the initial period. This implies the use of normal finite difference equations during the unstable initial period. Finally, as far as relevant cross sections are available, the calculation system can be extended to multi-group energy equations.

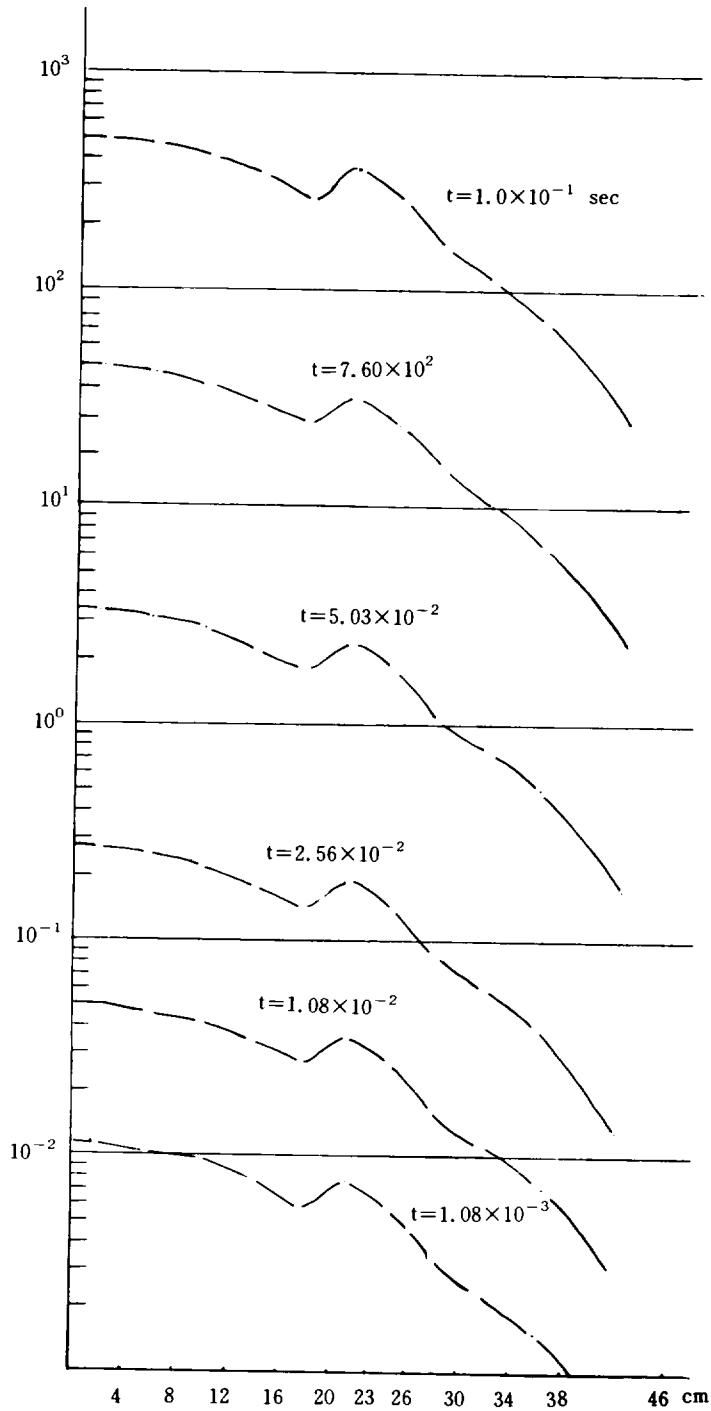


Fig.1. Thermal neutron flux transient.

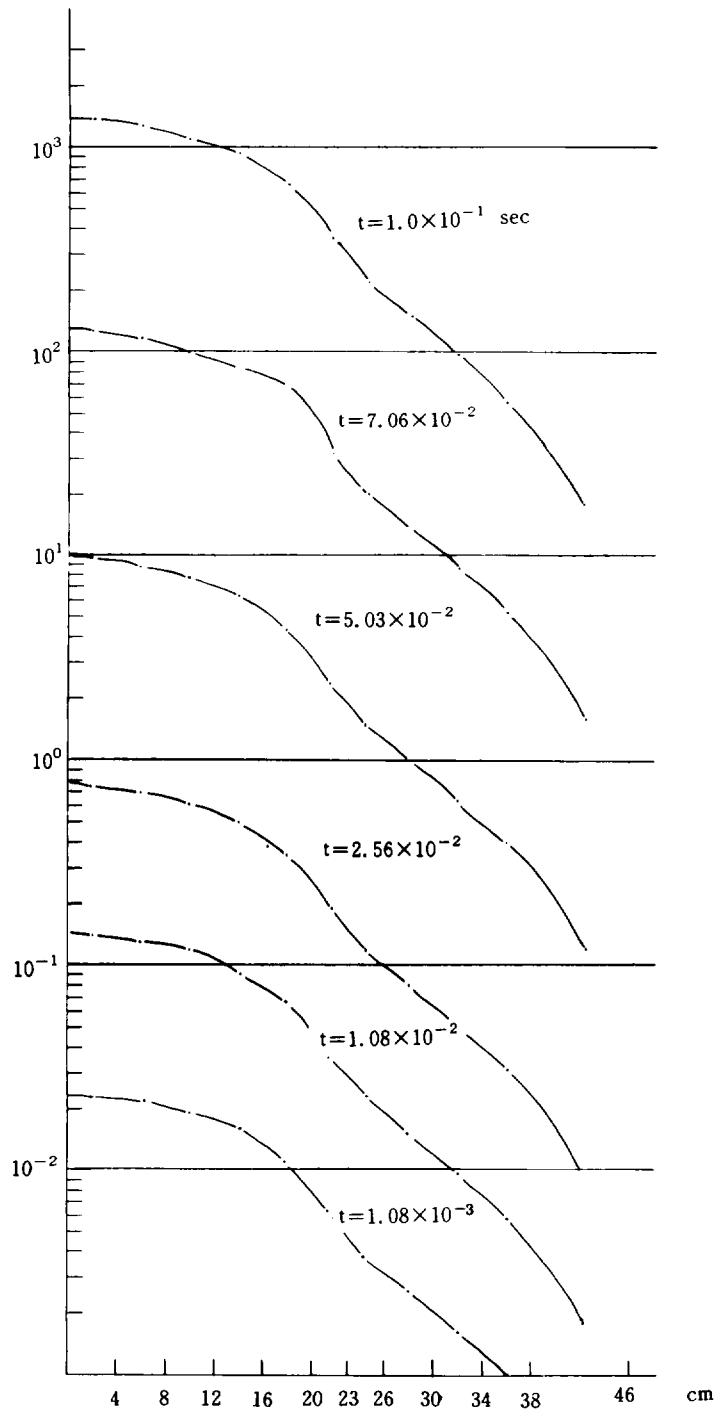


Fig.2. Fast neutron flux transient



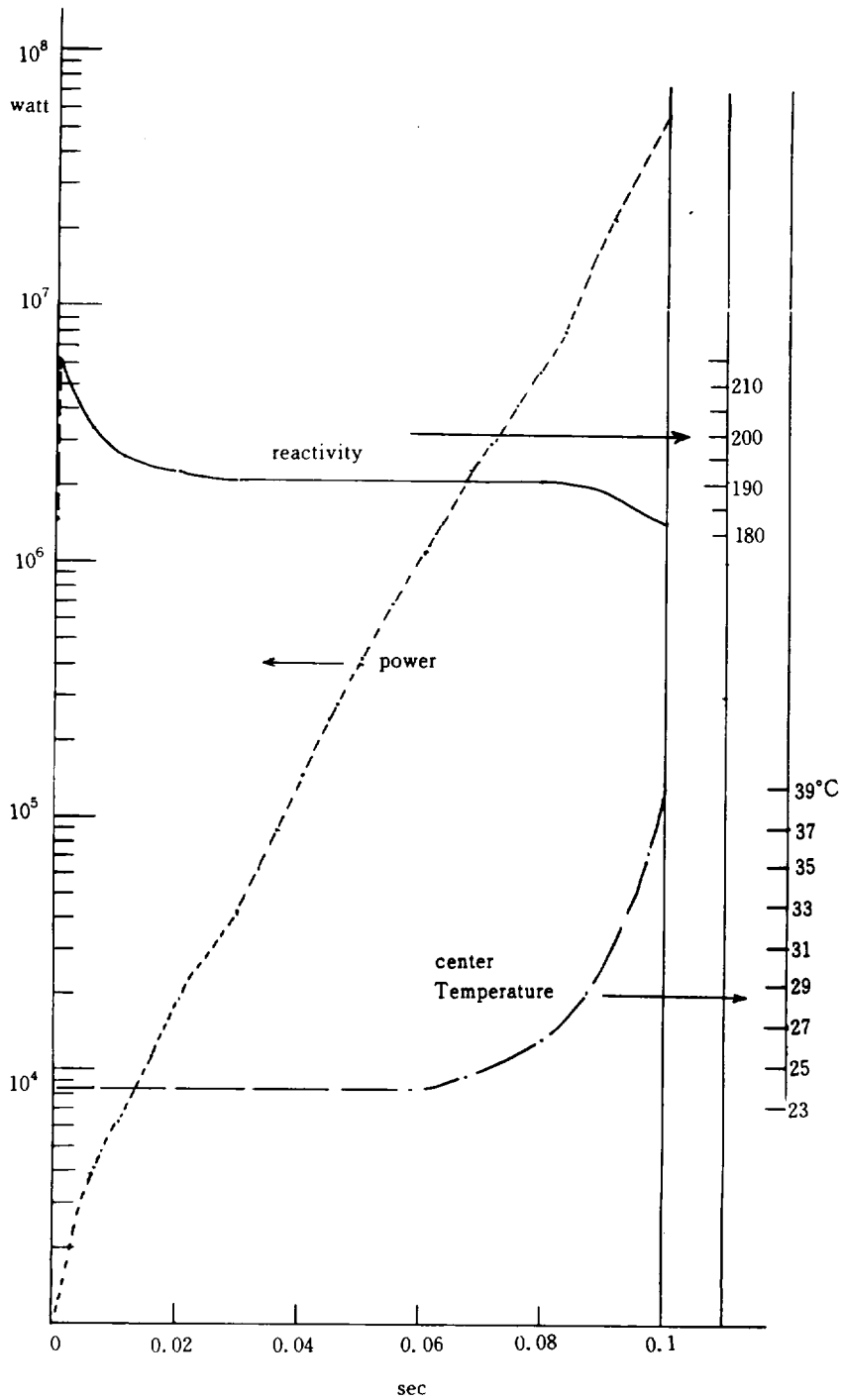


Fig. 3. Time vs. power, center temperature and reactivity

### Literature Cited

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### 국 문 초 록

중성자의 동특성해석을 위하여 시간 및 공간에 대한 비선형식을 컴퓨터 프로그램으로 작성하여 반응도 변화에 따른 시스템의 중성자속의 변화, 온도변화등을 검토하였다. 에너지에 대해서는 2군 에너지식을 사용하였으며 특히 계산 속도의 증가를 위해 시간 간격을 조절시킬 수 있도록 오차처리에 중점을 두었다.