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Prompt Alpha Calculation With Monte Carlo Code JMCT

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Abstract – *Two prompt alpha algorithms namely k_{eff}-α and α iteration are integrated into neutron-photon transport code JMCT. The Godiva-like test cases with different criticalities and neutron spectra types are calculated based on ENDF/B-VII.0 data. Results of TART and Tripoli-4 Monte Carlo codes are introduced as reference.*

I. INTRODUCTION

Prompt alpha is an important parameter describing neutrons' evolution in fissionable systems. It can be either measured from experiment or calculated by simulation. The experimental measures include Pulsed Neutron Source (PNS) [1], Rossi-α [2], and Feynman-α [3]. While for the numerical simulation, there are two kinds of methods which are dynamic-α and static-α methods.

The experimental methods are limited in many aspects. Take Rossi-α method for example. It is only available for systems at or very close to delayed critical in theoretical. This limitation cannot be overcome by experimental means. As for PNS method, experimental restrictions must be considered. The experiment on super-critical system is not practical. On the other hand, if the system is too sub-critical, the reaction rate is too low to be detected.

Numerical simulation is also widely used in researches. Usually, neutron transport equation can be solved with Monte Carlo method in alpha calculation. Dynamic-α method is based on time dependent fixed source neutron transport problem. Neutron flux are tallied by time steps and then fitted according to the exponential relation. The simplest example is the direct MC simulation of PNS experiment. The limitations of PNS experiment can be avoided by MC technique such as neutron population controlling. The most well-known MC code using this dynamic-α method is TART [4].

Although dynamic-α method can calculate fissionable systems with different criticalities, it is usually too time consuming because several calculations on different time steps are necessary. Comparing with dynamic-α, static-α method is more efficient. The alpha eigenvalue neutron transport equation is used to describe system's long period behavior. The long period here means long enough for neutron flux increasing (for super-critical system) or decreasing (for sub-critical system) by fundamental mode, but not so long when delayed neutron must be considered. Generally, the period is much longer in thermal system than that in fast system.

There are several strategies in the implement of static-α algorithm. k_{eff}-α implement is equipped by MCNP-4C [5] code and serpent [6] code. It takes advantage of the population controlling of k_{eff} iteration, but fatal error often happens in the calculation of sub-critical system. In sub-critical system, additional cross section proportional to 1/v is introduced as neutron production. Thermal neutrons may produce large number of descendants, and make the iteration instable. Improved iteration scheme has been proposed by Ye et al [7], which introduces additional absorption terms in both side of the equation. Andrea Zoia et al modifies this scheme further and adopts it in Tripoli-4 [8] code. However, a parameter in above iteration scheme must be pre-defined, and it still works badly in systems with large sub-criticality.

Another strategy is alpha iteration algorithm proposed by Hyung Jin Shim et al [9]. In this scheme, time source is generated between iterations. No other eigenvalue than α is introduced and neutron population controlling is imposed on time source directly. Therefore, anomalous termination can be avoided. It has been used in the calculation successfully on very sub-critical system with prompt k_{eff} ~ 0.15. Because all fission neutrons are simulated within one generation, it is time consuming in the calculation on near-critical systems. What's more, many time source neutrons inherit the same properties of their ancestors. The strong correlation between time source neutrons may influence the convergence of the iteration.

There are also other methods except dynamic-α and static-α. According to the point kinetics, alpha can be expressed as

$$\alpha_x = \frac{\rho_x - \beta_x}{\Lambda_x} \tag{1}$$

In equation (1), x represents the type of eigenvalue. Multiplication, collision and leakage eigenvalues are studied by Brian C. Kiedrowski [10] on several benchmarks. When multiplication eigenvalue k_{eff} is involved, it is actually a simulation of Rossi-α experiment. It should be noticed that only at or very close to criticality, these methods can give accurate result. For far from critical systems, this method may give wrong results.

II. ALGORITHM AND IMPLEMENTATION

In this work, k_{eff}-α and alpha iteration schemes are implemented into JMCT [11] code. A positive initial alpha guess switches JMCT to k_{eff}-α iteration branch for super-critical and near-critical systems. While negative initial alpha guess switches JMCT to alpha iteration branch for very sub-critical systems.

1. $K_{eff\text{-}\alpha}$ iteration

JMCT adopts the weight correction scheme proposed by Yamamoto [12,13] in the k_{eff}-α iteration implementation. It minimizes the modification of the original k_{eff} calculation flow. Time absorption or production is treated as a technique just like Russian roulette. When neutron flies a length *l*, the weight *w* is changed as follows,

$$w = w_0 \exp\left(-l \frac{\alpha}{v(E)}\right) \tag{2}$$

In equation (2), w_0 is the initial weight. All track length estimations remain unchanged except using averaged weight instead. The average weight during a track *l* is

$$w_a = \frac{1}{l}\int_0^l w_0 \exp\left(-l' \frac{\alpha}{v(E)}\right) dl' \tag{3}$$

If the system is very sub-critical, the exponential function shows an increasing of the neutron weight. This may be dramatic for the thermal neutrons which have small velocities, leading a large amount of fission neutron source produced in k_{eff}-α iteration scheme.

According to the α eigenvalue equation, α in the next generation can be calculated as,

$$\alpha^{i+1} = \alpha^{i}\left(1 + \frac{1}{\sum_j \Delta w_j}\left(N - \sum_j v_p \Sigma_f w_a l_j\right)\right) \tag{4}$$

N is the total source neutron weight at the start of the generation. Δw_j is the weight change during *j*-th segment of the random walk. v_p is neutron multiplication by prompt fission only.

2. Alpha iteration

K_{eff}-α iteration scheme has difficulties in the calculation of fissionable systems with large sub-criticality. Alpha iteration scheme proposed by Hyung Jin Shim is also adopted in JMCT code.

Alpha iteration scheme is similar to k_{eff} iteration. Within one k_{eff} generation, fission is treated as absorption, and the fission neutrons are produced as source of the next generation. However, in the case of alpha iteration, all the prompt fission neutrons are tracked within the generation, and time source neutrons are produced instead.

The cross section of time production is α/v, so the time source neutrons can be estimated using collision estimation as follows

$$N_{ijk} = \left\lfloor \left|\alpha^{i-1}\right| \frac{w_{ijk}}{v(E_{ijk})\Sigma_t} + \xi \right\rfloor \tag{5}$$

In order to control the population of time source, normalization can be done at the beginning of the next generation. The weight of time source in i+1 th generation is calculated by

$$w_{i+1} = \frac{N}{\sum_{jk} N_{ijk}} \tag{6}$$

Alpha can be estimated using collision, absorption or track length estimator just like k_{eff}. However, more inactive iterations may be needed considering the strong correlation of the time source between generations.

III. RESULTS

The Godiva-like problems proposed by Dermott et al. [14] are calculated by JMCT. Some results of TRIPOLI-4 [8] and TART [4] are also used as reference. In the following problems, ENDF/B-VII.0 is used in JMCT except when it is claimed explicitly.

1. Godiva-I

Godiva-I is a fast-critical system. It has a simple geometry which is a bare sphere with radius 8.74 cm. The material is U composed of ^{235}U, ^{238}U and ^{234}U with atom fraction 93.7695%, 5.2053% and 1.0252% respectively. The total density of the fuel is 18.7398 g/cm^3. The results of Godiva-I problem are shown in Table I.

Table I. Results of Godiva-I

	alpha(μs^{-1})	k_{eff}
JMCT k_{eff}-α	-1.179	0.99342
JMCT alpha	-1.162	-
TRIPOLI-4	-1.090	0.99349
TART	-0.739	0.99580
EXP	-1.1	-

30,000 neutrons per generation are simulated with 1500 inactive generations and 3500 total generations. Two alpha results of JMCT from different iteration scheme both show good agreement with TRIPOLI-4. TRIPOLI-4 also used ENDF/B-VII.0 database. But they are larger than result of TART in negative direction. Andrea Zoia et al. explained this discrepancy as the result of using different cross section data. For systems near critical, equation (1) can be changed with the form α = (k_{eff}-1)/Λ, where Λ is neutron generation time. In Godiva-I, Λ's value is about 0.006 μs [14]. Therefore, small difference in k_{eff} can lead significant deviation in α. It should be noted that the measured alpha value is about -1.1 μs^{-1} [15], showing a better agreement with results using ENDF/B-VII.0.

Neutron spectra are shown in Fig. 1. All the three curves are normalized to 1.0. The results agree well with each other at higher energies. However, the differences are significant at energies lower than 100 eV. Actually, most fluxes at low energies converge badly with statistical error larger than 0.2. Because Godiva-I is a fast system, neutrons are seldom thermalized. The total fraction of the neutrons lower than 100eV is less than 0.0001%. In the alpha iteration scheme, thermal neutron will produce a lot of time source in the next generation. Considering their strong correlations, the statistical error may be underestimated.

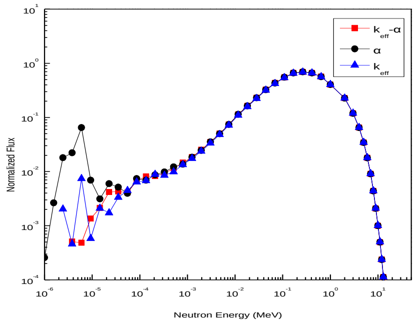

Fig. 1. Neutron spectra of Godiva-I problem

2. Godiva-II

In Godiva-II problem, all the configurations are same with Godiva-I except that the density is doubled to 37.4796 g/cm^3. For this super-critical system, only k_{eff}-α calculation is performed. The result is shown in Table II.

Table II. Results of Godiva-II

	alpha(μs^{-1})	k_{eff}
JMCT k_{eff}-α	145.13	1.58386
TRIPOLI-4	144.9	1.58455
TART	144.7	1.582

In this problem, 3,000 neutrons per generation, with 200 inactive generations and 500 total generations are simulated. JMCT k_{eff}-α gives a result closed to TRIPOLI-4 and TART. The comparison is shown in Fig. 2 for the k_{eff}-α and k_{eff} neutron spectra.

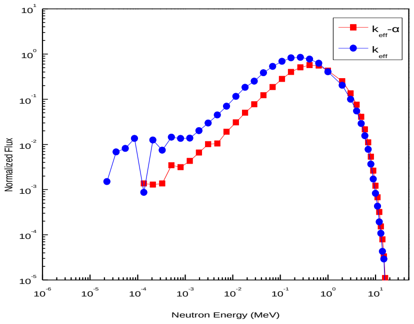

Fig. 2. Neutron spectra of Godiva-II problem

As for k_{eff}, neutrons below 100keV contribute 5.0% to the total flux. But it is less than 2.0% for k_{eff}-α. Because all the curves are normalized to 1.0, difference also exists at high energies. This is veiled by the log-log axis scale.

3. Godiva-III

Godiva-III adds a water sphere with 30 cm radius outside the uranium sphere based on Godiva-II. This configuration makes the system heterogeneous in space. The fission in the inner sphere is much faster than thermalization in the outer sphere. When thermal neutrons are reflected from the outer sphere, tremendous fast neutrons have been produced in the inner sphere by fission. Therefore, the neutron spectrum is fast. The results are shown in Table III.

Table III. Results of Godiva-III

	alpha(μs^{-1})	k_{eff}
JMCT k_{eff}-α	147.01	1.6802
TRIPOLI-4	146.9	1.66782
TART	146.6	1.661

For this system, the k_{eff} calculation solves another problem, in which the fission multiplication is reduced by a factor of k_{eff}. This difference can be found from neutron spectra comparison shown in Fig. 3.

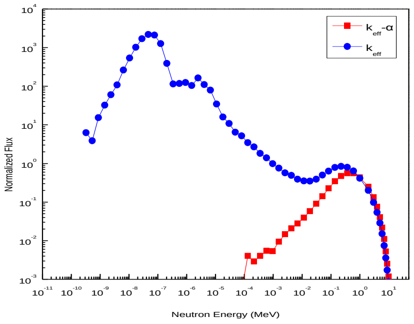

Fig. 3. Neutron spectra of Godiva-III problem

4. Godiva-IV

Godiva-IV adds 100% H_2O in atomic fraction into U sphere homogeneously. This makes it a thermal fission system. Similar test is done as Godiva I – III. The results are shown in Table IV and Fig. 4.

Table IV. Results of Godiva-IV

	alpha(μs^{-1})	k_{eff}
JMCT k_{eff}-α	0.6713	1.80519
TRIPOLI-4	0.671	1.79282
TART	0.653	1.771

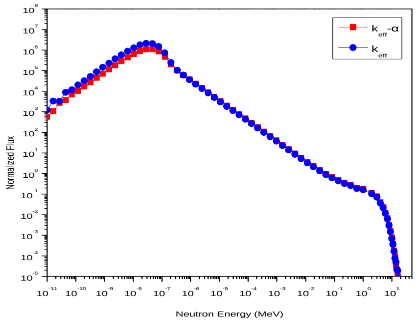

Fig. 4. Neutron spectra of Godiva-IV problem

The difference between k_{eff}-α and results k_{eff} is very small. This represents a special situation that k_{eff} gives the accurate result with a wrong solving process. Cullen et al. [4] explains that fast neutrons produced by fission are far less than thermal neutrons. Although fission multiplication is reduced by a factor of k_{eff}, little change in neutron spectrum happens.

5. Godiva-V

Godiva-V problem is a fast system with a large sub-criticality. It halves U's density based on Godiva-I. Alpha-iteration scheme is used in JMCT. The results are shown in Table V and Fig. 5.

Table V. Results of Godiva-V

	alpha(μs^{-1})	k_{eff}
JMCT alpha	-0.9397	0.52594
TRIPOLI-4	-0.979	0.52542
TART	-0.739	0.528

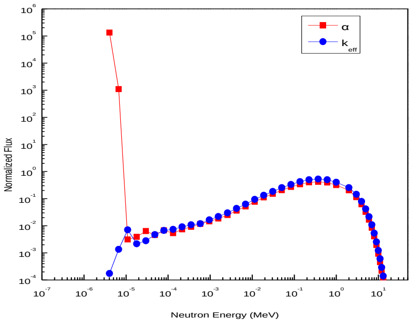

Fig. 5. Neutron spectra of Godiva-V problem

The spike at low energies is mainly determined by leakage. For simplicity, we consider a system with a void sphere with no fission or scattering happens. The alpha eigenvalue equation can be expressed as

$$\Omega \cdot \nabla\phi = -\frac{\alpha}{V}\phi \tag{7}$$

The flux in arbitrary position inside the sphere takes the following form

$$\phi = c_1 e^{\frac{c_2}{V}} \tag{8}$$

Parameters c_1 and c_2 are positive. Therefore, an exponentially decrease happens at low energy.

IV. CONCLUSIONS

Two iteration schemes are implemented into JMCT code. The test on Godiva-like benchmarks shows that the algorithm can be used in fissionable systems with different criticalities. Researches on source convergence of alpha iteration scheme still needs more efforts.

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