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The Three-Dimensional Continuously Varying Material Transport Method Based on RMC Code

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Abstract

Studying the continuously material model appropriate for liquid fuel reactor is important in order to properly take into account the physical properties of fuel solution in Monte Carlo transport calculation of fuel solution reactor. In this paper, the continuously varying material transport(cvmt) method using Direct Sampling is proposed in rector Monte Carlo code RMC. And a new numerical integration method for three-dimensional space is presented. And we mixed the Direct Sampling together with the RayTracking in our implementation. A three-dimensional fuel rod model is used to determine the correctness of this method compared with finely layered uniform material. The results of the calculations for uniform material and continuous material are closer the finer the meshing.

KeyWords: cvmt method, Direct Sampling, mixed transport, three-dimensional numerical integration method

1. Introduction

The fuel solution is in a complicated temperature field and flow field environment during the liquid fuel reactor's power operation, and its physical property parameters can be thought of as undergoing continual modifications. Studying the continuum model appropriate for liquid fuel reactor is important in order to carefully take into account the physical parameters of the fuel solution in the Monte Carlo transport calculation of fuel solution reactor[1].

Accuracy and processing efficiency cannot be guaranteed at the same time if the processing method of regional subdivision plus average temperature or cross section is employed for approximation. The continuously material, which offers precise and effective analysis for some advanced and novel concept reactors, such as solution reactors and supercritical water cooled reactors, can be used to directly simulate this type of problem[2].

In this paper, the continuously varying material transport(cvmt) method[3-4] is proposed in rector Monte Carlo code RMC[5]. And a new numerical integration method for three-dimensional space is presented. What's more, in order to make the transport method more general, the Direct Sampling method is mixed with the RayTracking method as the mixed-transport method in the RMC code.

Based on RMC code, we establish the three-dimensional cvmt method, the three-dimensional numerical integration method and the mixed-transport method in section 2. The cvmt method and numerical integration method are verified and validated in Section 3. Finally comes the conclusions in Section 4.

2. Methods' Methodology

This section will introduce the three-dimensional continuously varying material transport method, the numerical integration method and the mixed-transport method.

Firstly, we need to go through the particle transport method of Monte Carlo method .

2.1 Particle Transport Method and RayTracking

Neutrons and photons don't change the direction during flight, so the transport process only needs to sample their flight distance.

Given a grid element of fixed composition, the initial position of neutrons is s, and the probability of the first collision when neutrons travel in the direction of flight away from the element ds $p(s)ds$ is as Eq(1).

$$p(s)ds = e^{-\Sigma_t s}\Sigma_t ds \tag{1}$$

In Eq(1), Σ_t is the total cross section.

By integrating Eq(1), we can get the probability of reaction or collision when the neutron flies the distance l as Eq(2).

$$\xi = \int_0^l e^{-\Sigma_t s}\Sigma_t ds = 1 - e^{-\Sigma_t l} \tag{2}$$

Since $\xi \in (0,1)$, sampling the random number ξ from$(0,1)$, the neutron flight distance can be calculated as Eq(3).

$$l = -\frac{1}{\Sigma_t} ln(1-\xi) = -\frac{1}{\Sigma_t} ln(\xi) \tag{3}$$

In our RMC code, we use RayTracking to simulate the particle transport process, it is a method of determining the flight distance and the location of the collision point by considering whether neutrons collide in the layer medium.

For the material area shown in Figure 1, the RayTracking method is as the following steps.

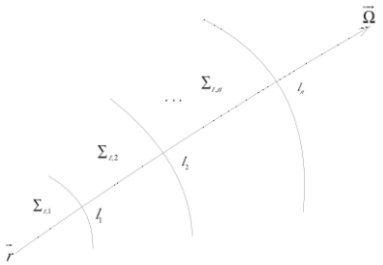

Fig.1 Material area of RayTracking

1) Firstly consider the first layer material, the use of the macroscopic cross section of material 1 $\Sigma_{t,1}$, select a random number ξ_1. The flight distances of particles are sampled in the $\Sigma_{t,1}e^{-\Sigma_{t,1}l}$ distribution as $l = -\frac{1}{\Sigma_{t,1}}ln(\xi_1)$.

2) If $l < l_1$, then it is believed that neutrons collide in the first material and travel a distance of l.

2) If $l > l_1$, then it is considered that neutrons do not collide in the first layer of medium, and the simulated point is moved to the junction of material 1 and material 2, and then sampling is carried out from the second layer of material until the final collision position is determined and the corresponding flight distance is obtained.

From the introduction of RayTracking method we can know that this transport method can't be used in the cvmt method. Because there is no concept of layering in the cvmt method.

To solve this problem, we use the Direct-Sampling method[6] introduced in section 2.2.

2.2 Direct-Sampling Method

The main difficulty of non-uniform continuous medium is the random sampling of the free flight distance of particles in the medium. In the process of particle flight, the cross section of the medium changes, that is, the equation of particle flight distance s is as Eq(4).

$$\xi = \int_0^x \Sigma(x)e^{-\int_{x_0}^{x}\Sigma(x')dx'}dx \tag{4}$$

In Eq(4), $\Sigma(x)$ is the total cross section along the x direction.

We define $\tau(x) = \int_0^x \Sigma(x)dx$ is the distance the particle travels through the medium, and define $P_{NC} = e^{-\tau(b)}$ is the non-collision probability.

The probability density function of particles colliding after moving x distance in the medium is shown as Eq(5).

$$\begin{aligned} f(x) &= P_{NC}\delta(x=\infty) + (1-P_{NC})\frac{1}{G}\frac{d\tau}{dx}e^{-\tau(x)} \\ &= P_{NC}\delta(x=\infty) + (1-P_{NC})g(x) \end{aligned} \tag{5}$$

In Eq(5), $\frac{d\tau}{dx}$ is the probability of collision per unit flight distance, and $e^{-\tau(x)}$ is the probability of non-collision after the flight distance x.

We can get Direct-Sampling method as the following steps in Fig.2.

```
Compute P_NC
Sample ξ1
if ξ1 <= P_NC then
    Move particle to cell boundary
else
    Sample ξ2
    Compute τ̂ = − ln[1 − (1 − P_NC)ξ2]
    Select s0
    n = 0
    while |sn − sn−1| < ε do
        n = n + 1
        g = τ̂ − τ̂(sn−1)
        g′ = dg/ds = −Σ(x0 + sn−1)
        sn = sn−1 − g/g′
    Move particle distance sn along flight path
```

Fig.2 The Algorithm of the cvmt method

From Fig.2 we use the Newton's method to get the fly-distance of a particle. However, it is very difficult to calculate $\tau(l) = \int_0^l \Sigma(x)dx$.

In one-dimensional space, the cross-section $\Sigma(x)$ is defined as Eq(6). Here $P_n(x)$ is the Legendre polynomial and $f(x)$ is a coordinate transformation function.

$$\begin{aligned} \Sigma(x) &= \sum_{n=0}^{N}\frac{2n+1}{2}b_nP_n\big(f(x)\big), \\ f(x) &= 2\left[\frac{x-x_{min}}{x_{max}-x_{min}}\right] - 1 \end{aligned} \tag{6}$$

So that in three-dimensional, it is very difficult to calculate $\tau(l)$.

In order to solve this problem, we proposed a new three-dimensional numerical integration method is section 2.3.

2.3 Three-Dimensional Numerical Integration Method

For three-dimensional, $\tau(x_0, y_0, z_0)$ is shown as Eq(6).

$$\tau(x_0, y_0, z_0) = \int_0^{z_0}\int_0^{y_0}\int_0^{x_0}\Sigma(x, y, z)dxdydz \tag{6}$$

Firstly, for the integration of this three-dimensional space, we don't use the coordinates x, y, z for integration, but use the particle's flight path s, which can be converted into a one-dimensional numerical integral of the independent variable s.

Secondly, according to the flight path of the particle, the flight path s is segmented $(2n+1)$, the cross section of each point $(2n+1)$, is obtained, and the quadratic equation is fitted using the Newton-Cott method, and the quadratic equation is calculated for every three points. It is shown as Eq(7).

$$\begin{aligned} \Sigma(s) &= as^2 + bs + c, s = s' + s_n \\ \Sigma(s' + s_n) &= p(s')^2 + qs' + m \\ m &= \Sigma(s_n) \\ q &= \frac{4\Sigma(s_{n+1}) - \Sigma(s_{n+2}) - 3m}{2\Delta s} \\ p &= \frac{\Sigma(s_{n+2}) - m - 2q\Delta s}{4\Delta s^2} \end{aligned} \tag{7}$$

In Eq(7), because the coefficients of the function can be expressed numerically by the function itself, no fitting calculation is required.

The Simpson's Law is as Eq(8).

$$\int_a^b f(x)dx = \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \quad (8)$$

Put Eq(7) into Eq(8), the integrals can also be expressed by using the principles of Simpson's Law as Eq(9) and can be calculated without fitting.

$$\int_{s_n}^{s_{n+2}} \Sigma(s)ds = \frac{\Delta s}{3}[\Sigma(s_n) + 4\Sigma(s_{n+1}) + \Sigma(s_{n+2})] \quad (9)$$

In Eq(9), s_n is the n segment track after the track s is divided into N segments.

With Eq(9), we can get a new algorithm[7] of the Direct-Sampling method as the following steps in Fig.3.

1: Sample N equally spaced Σ_t values along neutron flight path
2: Compute $\tau(s_b)$ using Newton-Cotes numerical integration
3: Compute $P_{NC} = exp[-\tau(s_b)]$
4: Sample ξ_1
5: **if** $\xi_1 \leq P_{NC}$ **then**
6: Move particle to cell boundary
7: **else**
8: Sample ξ_2
9: Compute $\hat{\tau} = -\ln[1-(1-P_{NC})\xi_2]$
10: $n = 1$
11: $\tau = 0$
12: **while** $\tau \leq \hat{\tau}$ and $n \leq N$ **do**
13: $\tau = \tau + \frac{\Delta s}{3}[\Sigma_t(s_n) + 4\Sigma_t(s_{n+1}) + \Sigma_t(s_{n+2})]$
14: $n = n + 2$
15: n = n - 2
16: $\tau = \tau - \frac{\Delta s}{3}[\Sigma_t(s_n) + 4\Sigma_t(s_{n+1}) + \Sigma_t(x_{s+2})]$
17: $\delta\tau = \hat{\tau} - \tau$
18: Calculate polynomial coefficients a, b, c using $\Sigma_t(s_n), \Sigma_t(s_{n+1}), \Sigma_t(s_{n+2})$
19: Invert $\frac{1}{3}a(s')^3 + \frac{1}{2}b(s')^2 + c(s') = \delta\tau$
20: Move particle distance $(n-1)\Delta s + s'$ along flight path

Fig.3 The new Algorithm of the cvmt method

2.4 The Mixed-transport Method

When we need to do the continuously varying material transport, we use the cvmt method based on the direct sampling. And when we need to do the layered uniform material transport, we use the RayTracking method. So when a case has both continuously varying material region and layered uniform material region, we implement the mixed-transport method that mixes the two transport methods.

For the material area shown in Figure 4, the mixed-transport method is as the following steps.

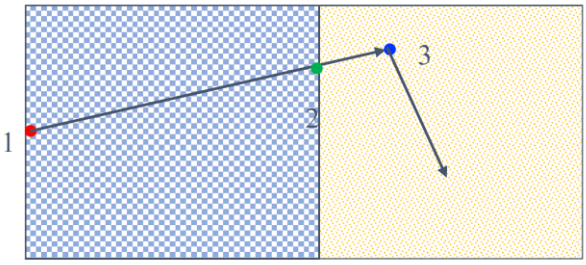

Fig.4 Material area of mixed-transport method

The mixed-transport method consider layer by layer whether neutrons collide in the layer material and determine the properties of the material (whether it is a continuous material) to determine which transport method to use.

1) Direct-Sampling is used for continuous material, and Raytracking is used for non-continuous material. What's more, we can determine the flight distance and collision point location.

2) If the particles didn't move to the boundary of the material, the neutrons are considered to have collided in the first layer of the material, the flight distance is obtained, and the same transport method will be continued using.

2) If the particle has moved to the boundary of the material, it is considered that neutrons didn't collide in the first layer of material, and the simulated point is moved to the junction of material 1 and material 2, and then sampling is carried out from the second layer of material (re-judging the material properties and selecting the transport method) until the final collision position is determined and the corresponding flight distance is obtained.

3. Methods Verification and Validation

This section tests the cvmt method with a fuel rod case, and compared the results with the layered uniform material. And the new three-dimensional numerical integration method is also tested.

3.1 Test of the Three-Dimensional Numerical Integration Method

In section 2.3 we get a new three-dimensional numerical integration method, but it need to cut the flight path s to $(2n+1)$ segments. So how to choose the variable n is a problem.

In general, the variable n is sufficient to be 11, for complex examples with drastic changes, n may need to be 101. We test the integration method with different functions and different variable n, the results is shown in Table I and Table II. The error comparison between numerical integration results and analytical solutions are shown.

Table I: Error comparison between numerical integration results and analytical solutions of simple functions

Function	3 segments	11 segments	101 segments	1001 segments
Constant	0%	0%	0%	0%
Primary function	0%	0%	0%	0%
Quadratic function	0%	0%	0%	0%
Cubic function	0%	0%	0%	0%

Table II: Error comparison between numerical integration results and analytical solutions of complexity functions

Function	3 segments	11 segments	101 segments
Quartic function	66.667%	0.107%	0%
Complexity functions $f(x) = e^x + \cos(x)$	0.629%	0.001%	0%
Integral along the axial path ternary quartic function	66.667%	0.107%	0%
Integral along three-dimensional path ternary quartic function	66.667%	0.107%	0%
three-dimensional ternary quartic function	66.667%	0.107%	0%

In the test in Table II, x represents the length in one-dimensional direction, and x_0 is the origin point.

From Table I we can see that for the simple functions, such as the primary function and the quadratic function, no matter how many segments are divided, the calculation error between numerical integration results and analytical solutions are less than 0.00001, which can be ignored. So that, for the simple functions, the variable n is sufficient to be 3 or 11.

From Table II we know that for the complexity functions, such as quartic function and ternary quartic function, the error is very large when divided into 3 segments. When dividing into 11 segments, the error is about 0.1%, which can meet some calculation requirements. If you want to get more accurate results, it need to increase the number of segments to 101. And for three-dimensional ternary quartic function, 101 segments can also get a n accurate result.

Therefore, we use 101 segments for the cvmt method.

3.2 Test of the cvmt Method

A fuel rod case is used to test the cvmt method, and the results will be compared with different uniform material which divided into different segments to prove the correctness of this method. The radial diagram of the fuel rod is shown in Figure.5 and 6.

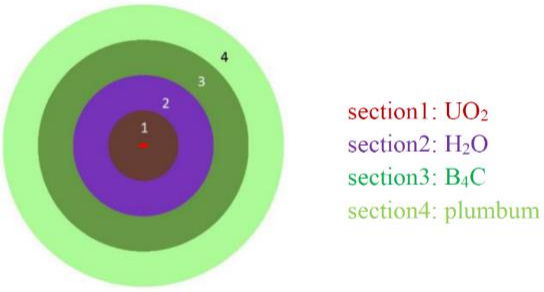

Fig.5 Radial diagram of the fuel rod

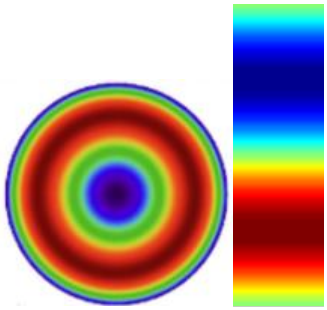

Fig.6 continues material distribution of test case in radial and axial direction

This is the XY cross section of the fuel rod. The materials for regions 1, 2, 3 and 4 are UO_2, H_2O, B_4C and plumbum. In addition, the radius are 10 cm, 20 cm, 30 cm and 40 cm. The height of the cylinder is 20 cm. And it is a continuous energy simulation case. The critical calculation is carried out in RMC, and the total number of simulated batches is 200 with 100 inactive batches. The number of particles per batch is 50000, and the simulation uses a 20-core MPI parallel. It is calculated with cvmt method and different segments uniform material. The results are shown in Table III.

Table III: Error comparison between cvmt results and different segments uniform material of different UO_2 density changing curves

UO_2 density changing curves	Calculation method	k-effective (Standard deviation)
Complex function varies along the vertical axis 4 order Legendre polynomial	cvmt	0.8276(0.0045)
	20 segments uniform material	0.8289(0.0015)
	8 segments uniform material	0.8495(0.0013)
	2 segments uniform material	0.9078(0.0014)
Complex function varies along the radial direction 4+0 order Zernike polynomial	cvmt	1.4053(0.0053)
	10 segments uniform material	1.4085(0.0021)
	4 segments uniform material	1.3745(0.0018)
	2 segments uniform material	1.3036(0.0021)
Complex function varies along the vertical axis 4 order Legendre polynomial and radial direction 4+0 order Zernike polynomial	cvmt	1.1543(0.0065)
	20+10 segments uniform material	1.1522(0.0034)
	8+4 segments uniform material	1.1876(0.0031)
	2+2 segments uniform material	1.2768(0.0033)

In Table III, because the axial length of the case is long, the segmentation needs to be denser in order to calculate accurate. However, the radial direction of the example is narrow, so the segmentation of 10 segments is enough to obtain the same accurate calculation results.

From Table III we know that for this continuously material case, the cvmt method has the most accuracy

result. For the layered uniform material results, when it is roughly divided into 2, 4 or 8 segments, the error will be large compared with the cvmt method. And the results of the calculations for uniform material and continuous material are closer the finer the meshing. However the finely layered uniform material will cost large computation time and memory occupied.

In addition, the cvmt method can be used in three-dimensional case which varies along the vertical axis 4 order Legendre polynomial and radial direction 4+0 order Zernike polynomial.

What's more, compared with the finely layered uniform material is to explain the correctness of the method. The cvmt method can offer precise and effective analysis for some advanced and novel concept reactors, such as solution reactors and supercritical water cooled reactors, can be used to directly simulate the continuously material problem.

4. Conclusions

In this paper, the continuously varying material transport(cvmt) method is proposed in RMC. And a new numerical integration method for three-dimensional space is presented. What's more, the Direct Sampling method is mixed with the RayTracking method as the mixed-transport method in the RMC code.

The following conclusions can be taken from the calculation results in section 3.

1. The results of the calculations for uniform material and continuous material are closer the finer the meshing.
2. The mixed-transport method can make the RayTracking method more general, and can improve the computational efficiency of cvmt method.
3. Compared with the finely layered uniform material is to explain the correctness of the method. The cvmt method can directly simulate the continuously material problem while layered uniform material can't.

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