Annals of Nuclear Energy 63 (2014) 491–498

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Development of a MCNP–ORIGEN burn-up calculation code system and its accuracy assessment

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ARTICLE INFO

Article history:
Received 9 April 2013
Received in revised form 8 August 2013
Accepted 9 August 2013
Available online 11 September 2013

Keywords:
MCNP
ORIGEN
Burn-up
VVER-1000 LEU
Fast reactor core

ABSTRACT

An MCNP–ORIGEN burn-up calculation code system, named MCORE (MCNP and ORIGEN burn-up Evaluation code), is developed in this work. MCORE makes use of the Monte Carlo neutron and photon transport code MCNP4C and nuclides depletion and decay calculation code ORIGEN2.1. MCNP and ORIGEN are coupled by data processing and linking subroutines. In MCORE, a so called "modified predictor corrector" approach is used. MCORE provides the capability of using different depletion calculation schemes and simulating fuel shuffling. Total nuclide density changes in active cells are considered in MCORE. The validity and applicability of the developed code are tested by investigating and predicting the neutronic and isotopic behavior of a "VVER-1000 LEU Assembly Computational Benchmark" at lattice level and a "Physics of Plutonium Recycling" fast reactor at core level (OECD-NEA).

The comparison results show that the MCORE code predicts the nuclide composition within 5% accuracy and k_∞ within 800 pcm at the end of the burn-up for LEU assembly (40 MWD/kg HM). For a fast reactor, the results obtained by MCORE are in the range of reported results except for ^{243}Am. In general, MCORE results show a good agreement with the benchmark values.

1. Introduction

In many nuclear applications such as fuel management and reactor core design, burn-up calculation is needed. Burn-up calculation aims at following the time development of material compositions and neutronics during reactor operations. In order to obtain accurate burn-up results, the neutron transport process should be simulated accurately by solving the Boltzmann transport equation. The analytical solution of the transport equation is very difficult for complex geometries.

The continuous-energy Monte Carlo method (Spanier and Gelbard, 1969) is one of the most reliable methods in the field of neutron transport problem because of its precise modeling of geometry and accurate modeling of physical phenomena. In the last couple of decades, its application has been expanded to burn-up problems (Jafarikia et al., 2010; Kelly, 1995; Morimoto et al., 1989; Okumura et al., 2000; Trellue and Poston, 1999) and it has shown a good practicability. If users have little calculation experiences or the geometry is quite complicated, the Monte Carlo method is very useful compared with conventional deterministic neutron transport codes. MCNP (Briesmeister, 2000) is the most widely used one among most existing standard multipurpose continuous energy Monte Carlo codes. MCNP can be used for calculations of multiplication factor, reaction rates, neutron fluxes, spectra etc.

In the past few decades, a number of Monte Carlo burn-up calculation code systems have been developed. Two kinds of calculation strategies have been used: (1) combining Monte Carlo code with an auxiliary modular code which has the function of depletion calculation, such as MVP-BURN (Okumura et al., 2000), MCB (Cetnar et al., 2002) and BURNCAL (Parma, 2002), and (2) coupling Monte Carlo code with a special depletion and decay calculation code by data processing and linking code, such as MOCUP (Moor et al., 1995), Monteburns (Trellue and Poston, 1999), ALEPH (Haeck and Verboomen, 2006) and IRBURN (Jafarikia et al., 2010). In the first kind of burn-up codes, the main approach is to use neutron absorption and fission reaction information to determine the nuclide composition at a next time step, which does not need post-processing and additional manipulation of neutron flux and cross-section set. In the second kind of burn-up codes, ORIGEN (Croff, 1983) is regularly used. ORIGEN is a versatile point depletion and decay calculation computer code.

MCNP4C and ORIGEN2.1 are coupled in the present work. The coupling code MCORE can make full use of the MCNP and ORIGEN codes for depletion and decay calculations of nuclides. In MCORE, "modified predictor corrector" approach is used, which can increase the time step and ensure enough accuracy. Fuel shuffling can be simulated after burn-up and decay calculation in MCORE. The code also provides the capability of using

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http://dx.doi.org/10.1016/j.anucene.2013.08.020

Nomenclature

E	neutron energy (eV)	n	nuclide subscript
F	fission density	t	time (s)
N	atomic density (at./b-cm)	w_f	effective energy released per fission (MeV/fission)
P	power of the system (MW)	Φ	absolute neutron flux of a burn-up zone (neutron/cm^2-s)
R	reaction rate (/cm^3-s)	γ	creation rate due to fission
V	volume (cm^3)	λ	creation rate due to capture
a, c, f	absorption, capture and fission subscript	$\bar{\nu}$	average number of neutrons released per fission
g	microscopic cross-section type subscript	σ	microscopic cross-section (barns)
i, j, k, l	isotope subscript	ϕ	neutron flux (neutron/cm^2-s)
k_{eff}	effective neutron multiplication factor		
m	cell subscript		

different depletion calculation schemes, which are determined by the user.

In this paper, the coupling of Monte Carlo code MCNP4C with burn-up code ORIGEN2.1 is presented. To evaluate the validity and applicability of the code system, a VVER-1000 LEU assembly and a fast reactor benchmark are calculated and compared.

2. Burn-up calculation method

2.1. Depletion and decay calculation

In reactor design burn-up calculations, the key objective is to determine the time-dependent fuel material compositions and eigenvalues as a function of burn-up. The rate of change in the concentration of a specific isotope is equal to its production rate per unit volume minus its removal rate per unit volume. A general expression for the formation and disappearance of a nuclide by nuclear transmutation and radioactive decay can be written as follows:

$$\frac{dN_i}{dt} = \sum_j \gamma_{ji}\sigma_{f,i}N_j\phi + \sum_k \sigma_{c,k\to i}N_k\phi + \sum_l \lambda_{l\to i}N_l - (\sigma_{f,i}N_i\phi + \sigma_{a,i}N_i\phi + \lambda_i N_i) \quad (1)$$

where $\frac{dN_i}{dt}$ is the rate of change in concentration of isotope i, $\sum_j \gamma_{ji}\sigma_{fj}N_j\phi$ is production rate per unit volume of isotope i from fission of all fissionable isotopes, $\sum_k \sigma_{c,k\to i}N_k\phi$ is production rate per unit volume of isotope i from neutron transmutation of all isotopes, $\sum_l \lambda_{l\to i}N_l$ is production rate per unit volume of isotope i from decay of all isotopes, $\sigma_{f,i}N_i\phi$ is removal rate per unit volume of isotope i by fission, $\sigma_{a,i}N_i\phi$ is removal rate per unit volume of isotope i by neutron absorption, $\lambda_i N_i$ is removal rate per unit volume of isotope i by decay.

In Eq. (1), the coefficients, such as continuous-energy cross-sections, are obviously not constant over the entire cycle. In order to solve this equation correctly, the cycle needs to be divided into a number of small time steps, during which the coefficients are assumed to be constant.

For a given nuclear system, the entire space can be divided into many cells. An execution of MCNP is possible if geometry and material compositions of each active cell are given. As a result of MCNP calculation, power, neutron flux and microscopic cross-sections of every nuclide in each active cell are calculated. On the other hand, ORIGEN execution for each cell is possible if the microscopic cross-sections and power or flux are given. Therefore, the coupling of a Monte Carlo code and a depletion calculation code can be directly realized only by implementing an interface program between them, which can simulate the nuclide depletion and decay in complicated geometries based on the capability of modeling complicated geometries by MCNP.

ORIGEN uses spectrum averaged one-group neutron cross-sections, which, as discussed above, are not constant during burn-up. Therefore, in order to calculate the depletion and decay of nuclides over an entire cycle correctly, cross-section library of ORIGEN should be modified and updated. ORIGEN provides the function of updating the cross-section library (LPU command and TAPE3 input file).

2.2. Power distribution and neutron flux calculation

ORIGEN provides two modes of depletion schemes, constant power (IRP command) and constant flux (IRF command), which implies that either power or flux will be constant for each active cell in the internal time step. As mentioned above, Monte Carlo code MCNP can be used to calculate power distribution and neutron flux, which are the main input information of ORIGEN.

Fission density F in cell m can be calculated as follows:

$$F_m = \left(\int_{E_{\min}}^{E_{\max}} N\phi(E)\sigma_f(E)dE\right)_m \quad (2)$$

where N is nuclide density, $\phi(E)$ is energy-dependent flux (neutron/cm^2-s), $\sigma_f(E)$ is energy-dependent fission cross-section (barns), m is cell number. Since the power produced in one cell is linearly proportional to the number of fissions in that cell, power produced in each cell can be calculated by multiplying the system thermal power and the relative number of fissions in that cell. As the relative number of fissions in each cell is proportional to the fission density and the volume of that cell, we can obtain the power of each cell:

$$P_m = \frac{F_m V_m}{\sum_m F_m V_m} P \quad (3)$$

One-group neutron flux ϕ in each active cell is provided by MCNP flux tally F4 as:

$$\phi_m = \int \phi_m(E)dE \quad (4)$$

Since the neutron flux is normalized to one source neutron in MCNP, the results of Eq. (4) has to be properly normalized to obtain absolute neutron flux Φ. As long as we know the thermal power of the system, the absolute neutron flux of each active cell can be achieved as follows (Snoj, 2006):

$$\Phi_m = \frac{P\bar{\nu}}{1.6022\times 10^{-13} w_f}\frac{1}{k_{eff}}\phi_m \quad (5)$$

where P is the thermal power of the system (MW), $\bar{\nu}$ is average number of neutrons released per fission, w_f is effective energy released per fission(MeV/fission) and k_{eff} is the effective neutron multiplication factor.