Annals of Nuclear Energy 63 (2014) 371–381

Contents lists available at ScienceDirect

Annals of Nuclear Energy

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

Numerically stable Monte Carlo-burnup-thermal hydraulic coupling schemes

D. Kotlyar *, E. Shwageraus

Department of Nuclear Engineering, Ben-Gurion University, POB 653, Beer Sheva 84105, Israel

ARTICLE INFO

Article history:
Received 23 May 2013
Received in revised form 28 July 2013
Accepted 2 August 2013
Available online 30 August 2013

Keywords:
Monte Carlo
Depletion
Neutronic thermal hydraulic coupling
BGCore
Implicit method
SIMP

ABSTRACT

This paper presents stochastic implicit coupling method intended for use in Monte-Carlo (MC) based reactor analysis systems that include burnup and thermal hydraulic (TH) feedbacks. Both feedbacks are essential for accurate modeling of advanced reactor designs and analyses of associated fuel cycles. In particular, we investigate the effect of different burnup-TH coupling schemes on the numerical stability and accuracy of coupled MC calculations. First, we present the beginning of time step method which is the most commonly used. The accuracy of this method depends on the time step length and it is only conditionally stable. This work demonstrates that even for relatively short time steps, this method can be numerically unstable. Namely, the spatial distribution of neutronic and thermal hydraulic parameters, such as nuclide densities and temperatures, exhibit oscillatory behavior. To address the numerical stability issue, new implicit stochastic methods are proposed. The methods solve the depletion and TH problems simultaneously and use under-relaxation to speed up convergence. These methods are numerically stable and accurate even for relatively large time steps and require less computation time than the existing methods.

1. Introduction

Monte-Carlo (MC) neutron transport codes gain popularity in the reactor analysis applications due to their flexibility in simulating complex fuel and core geometries without any significant approximations. However, MC codes lack the ability to perform time-dependent burnup calculations and, therefore, must be coupled with external codes in order to perform fuel cycle analyses. A number of different methods to couple the MC and burnup codes have been suggested. The simplest and the most commonly used is the explicit predictor Euler method. It is used in many MC-burnup coupling programs and shown to produce accurate results in many practical applications, for example as shown in Bomboni et al. (2010). Among such coupled codes are MOCUP (Moore et al., 1995), MCODE (Xu et al., 2002), MONTEBURNS (Trellue, 2003), SERPENT (Leppänen, 2007), BGCore (Fridman et al., 2008b), MCNPX (Fensin et al., 2010) and many others.

Recent advances in high performance computing capabilities allow substantial reduction in execution time of such burnup-MC codes. This, in turn, enables consideration of problems with much higher degree of complexity, such as introduction of thermal hydraulic (TH) feedback into the calculation scheme. In several recent studies, coupled MC and TH codes were successfully applied to model fuel assembly and mini-core size problems. For example, a coupling scheme between MCNP (Briesmeister, 2000) and COBRA-TF (Basile et al., 1999) was reported in Sanchez et al. (2009), for the prediction of pin power distribution in a PWR fuel assembly. A coupled system MCNP5/SUBCHANFLOW was described in Ivanov et al. (2011). It was developed for the fuel pin and assembly wise simulation of LWRs as well as advanced reactors. However, in none of the studies mentioned above, the burnup and TH feedbacks were applied simultaneously. In a recent work, we reported on the development of a coupled code, BGCore, which is capable of performing both depletion and TH analyses. To demonstrate the capabilities of BGCore system, a coupled neutronic TH analysis of a full PWR core was performed and reported in Kotlyar et al. (2011). BGCore produced very good results closely matching those obtained with the state of the art 3D deterministic nodal diffusion code DYN3D (Grundmann et al., 2000).

The current analysis presents a new incremental step in the direction of fully coupled MC calculation with burnup and TH feedbacks. In addition, various coupling schemes are examined to assess their accuracy and numerical stability.

The simplest and the most commonly used approach is the beginning of time step (BOT) method. However, the explicit nature of this method makes it only conditionally stable. That is, in some problems, if the time step size used in the calculations is sufficiently large, the solution can be numerically instable. It was shown in Dufek and Hoogenboom (2009); Dufek et al. (2013a)

* Corresponding author. Tel.: +972 86472175.
E-mail address: kotlyar@bgu.ac.il (D. Kotlyar).

0306-4549/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.anucene.2013.08.016

and Kotlyar and Shwageraus (2013) that applying the BOT method to MC-burnup calculations may result in oscillatory behavior of the spatial flux distribution. To overcome the instability issues, implicit methods were proposed (Dufek et al., 2013b) to couple burnup with MC transport codes.

In the current work, we first show that similar instabilities exist in the BOT MC-burnup-TH coupling analyses. The BOT method with relatively short time steps is commonly adopted in deterministic codes because the neutron transport solution is relatively inexpensive from the computational resources point of view. On the other hand, in MC calculations, very short time steps may result in prohibitively high computational costs and, therefore, not practical for the fuel cycle analysis applications.

In order to address the issue of numerical stability, while keeping reasonably low computational costs, two alternative methods are proposed here. Both methods are referred to as stochastic implicit mid-point (SIMP) methods, which, as we will show, produce stable and accurate results for the studied test case. In contrast to traditional approach, where TH and burnup iterations are performed sequentially, in the proposed methods, the depletion and TH problems are solved simultaneously and iteratively with the transport problem. The iterative scheme uses a variable relaxation factor, known as step-size, based on the Robbins–Monro algorithm (1951). An example for the use of variable step-size in reactor analysis at steady state conditions can be found in Dufek and Gudowski (2006). Their work presented the coupling between neutron fluxes, obtained from MC transport calculations, and strong feedbacks, such as coolant density and Xe-135 fission product density.

The SIMP methods proposed here are intended to be applied to MC-burnup-TH coupling problems. As will be demonstrated, not only both methods are unconditionally stable, because of their implicit nature, they also allow using relatively large time steps in fuel cycle calculations with minimal effect on the accuracy of the results. Large time steps allow substantial reduction of computation time.

An additional feature of the proposed methods is in the approach for evaluating different quantities of interest, such as power and temperature distributions. In fuel depletion analysis, the nuclide densities are obtained at fixed time points (beginning and end of time steps). This is typically done by assuming that the spatial power distribution is constant during the time step and corresponds to some fixed point in time (usually beginning of time step). This assumption is not strictly true, especially if the time steps are relatively large. Furthermore, the assumption of constant power during the time step implies fixed TH conditions and also leads to neglecting the effect of changing neutron spectrum. Ideally, the depletion step should be performed using the "time step average" power, TH conditions and spectrum (cross sections) and *not* using these quantities at some fixed point in time, as done by most of the existing codes. Finding such "time step average" parameters necessary for performing the depletion step is the main innovative feature of the two methods discussed here.

As a test case, we performed depletion of a typical 17 × 17 PWR fuel assembly with reflective boundary conditions in the radial direction. The assembly was axially divided into multiple burnable and thermal hydraulic zones. This division was introduced in order to obtain detailed flux distribution and account for the depletion and TH conditions in each burnable region. The calculations were performed with BGCore reactor analysis system.

2. Description of BGCore code system

The proposed SIMP methods were programmed into the BGCore system. BGCore is a system of codes developed at Ben-Gurion University, in which Monte-Carlo code MCNP4C is coupled with fuel depletion and decay module SARAF. Data library for SARAF is based on JEFF-3.1 files (Koning et al., 2006). BGCore utilizes multi-group methodology for calculation of one group transmutation cross-sections (Haeck and Verboomen, 2007; Fridman et al., 2008a) which significantly improves the speed of burnup calculations. In addition to the depletion module, BGCore system also includes a TH feedbacks module – THERMO. The modules are executed iteratively so that the coupled system is capable of predicting fuel composition, power, coolant density and temperature distributions in various types of reactor systems.

3. Description of burnup-thermal hydraulic coupling methods

The objective of coupled burnup-TH analysis is to obtain the nuclide field $\mathbf{N}_F(\mathbf{r}, t)$ and the TH properties $N_T(\mathbf{r}, t)$ as a function of space and time. Knowing, $\mathbf{N}_F(\mathbf{r}, t)$ and $\mathbf{N}_T(\mathbf{r}, t)$ allows, then, to determine the spatial, energy and time dependent neutron flux$\phi(\mathbf{r},E,t)$. However, $\mathbf{N}_F(\mathbf{r}, t)$ and $\mathbf{N}_T(\mathbf{r}, t)$ themselves depend on $\phi(\mathbf{r},E,t)$. That is, $\phi(\mathbf{r},E,t)$ requires a prior knowledge of $\mathbf{N}_F(\mathbf{r}, t)$ and $\mathbf{N}_T(\mathbf{r}, t)$, which are both driven by the neutron flux. This non-linear problem can be described by three coupled equations. First one is the burnup equation that determines the nuclide field changes, as described in Eq. (1). The second is the heat balance equation that computes the temperature distribution from which also the coolant and/or moderator densities can be derived. The last is the neutron transport eigenvalue equation that provides the fundamental neutron flux mode:

$$\mathbf{N}(\mathbf{r}, t) = \exp[\mathrm{M}(\phi, T)(t - t_0)] \times \mathbf{N}(\mathbf{r}, t_0) \tag{1}$$

In Eq. (1), $\mathbf{N}(\mathbf{r}, t_0)$ describes the nuclide field at time t_0. The neutron flux $\phi(\mathbf{r},E, t)$ at time t is determined by the fundamental mode of the neutron transport equation and will be denoted here as "$\phi_{\mathbf{B}}$". In other words, the operator $\phi_{\mathbf{B}(\mathbf{N}_{F(\mathbf{r},t)},\mathbf{N}_{T(\mathbf{r},t)})}$ computes $\phi(\mathbf{r},E,t)$.

The operator **M** in Eq. (1) is described in following equation:

$$\mathrm{M}(\phi, T) = \int_0^\infty \phi(\mathbf{r}, E, t)\mathbf{X}(T)dE + D \tag{2}$$

where **X** is a cross section and fission yields matrix, D is a decay matrix, and $T(\mathbf{r},t)$ is the temperature at point **r** and time t. $T(\mathbf{r}, \mathrm{t})$ is obtained by solving heat conduction and convection problem and will be denoted here by the operator '**T**'. Consequently, the operator $T(\phi)$ computes $T(\mathbf{r},\mathrm{t})$.

There are various schemes to couple the burnup and TH feedbacks with the neutron transport equation. The most commonly used BOT method is based on dividing the entire irradiation time interval into "small" time step increments. Fixed time point TH iterations are performed at BOT until convergence on power distribution or reaction rates is achieved. Then, the space and energy dependent microscopic reaction rates are assumed to be constant during each time step. Knowing these reaction rates allows obtaining the concentration at the EOT in a single calculation step. This method is known as the explicit Euler method. The accuracy of the BOT method obviously depends on the time step length. Furthermore, it is only conditionally stable. As mentioned earlier, short time steps would require prohibitively high computational resources and, as a result, will be not practical in fuel cycle analysis.

Therefore, two alternative methods are proposed. Both methods are implicit in nature and therefore avoid the numerical oscillations. The implicit solution is obtained by using the so-called stochastic approximation. The mathematical derivation of the methods is presented in the following section along with the algorithms for each of the burnup-TH coupling procedures. The nomenclature is given in Table 1.