Annals of Nuclear Energy 88 (2016) 158–173

Contents lists available at ScienceDirect

Annals of Nuclear Energy

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

Uncertainty and global sensitivity analysis of neutron survival and extinction probabilities using polynomial chaos

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ARTICLE INFO

Article history:
Received 5 June 2015
Received in revised form 30 October 2015
Accepted 2 November 2015

Keywords:
Extinction probability
Backward Master equation
Polynomial chaos
Global sensitivity

ABSTRACT

Generalised Polynomial Chaos (GPC) in conjunction with sparse grid stochastic collocation and High Dimensional Model Representation (HDMR) is used to perform uncertainty and global sensitivity analysis for the neutron chain survival and extinction probabilities, with and without an intrinsic random source. Starting with a lumped backward Master equation formulation, uncertainty is introduced by allowing the factorial moments of the fission multiplicity distribution, the neutron lifetime, and strength of the intrinsic source to be independent and uniformly distributed random variables. A multidimensional Legendre chaos representation of the random survival and extinction probabilities is used to achieve optimal numerical convergence in the stochastic dimension and the relative variance contributions from each random parameter are then quantified using High Dimensional Model Representation (HDMR).

The underlying deterministic results of the model are found to closely match analytical benchmarks and, once uncertainty is introduced, the GPC results match both Monte Carlo simulations and analytical results for polynomial order greater than two. The GPC method is found to require significantly less computational time to achieve a given accuracy on the survival and extinction probabilities than the Monte Carlo method. It is found that, the probabilities are most sensitive to χ_i for lower i and have a significant sensitivity to χ_2 in all cases. A chain's survival probability is moderately sensitive to the neutron lifetime early in simulation. In the subcritical case this sensitivity increases as the simulation continues whilst it decreases in the supercritical case. The extinction probability is sensitive to the source strength.

1. Introduction

A vast body of work has been published to date on the probabilities of extinction, survival and divergence of the neutron population in a multiplying medium (Bell, 1963, 1965; Williams, 1974; Pazsit and Pal, 2008; Prinja and Souto, 2009, 2010; Prinja, 2012). These probabilities are key quantities in the characterization of strongly stochastic neutronic systems (exemplified by multiplying media with weak internal sources) where the fluctuations in the neutron number are large enough that low order statistical moments, such as the mean and variance of the neutron number, do not provide sufficient information to describe the instantaneous state of the neutron population and to predict its time evolution. Applications where such stochastic behavior is important include: criticality excursions in spent fuel storage, in the handling of fissile solutions in fuel fabrication and reprocessing; approach to critical under suboptimal reactor start-up conditions; preinitiation in fast burst research reactors; and weak nuclear signatures in the passive detection of nuclear materials. Especially from a safety viewpoint, it is clearly important to have an accurate estimate of the probability that a neutron chain will grow without bound.

The subject of stochastic neutron populations lends itself to an elegant and complete formulation based on the theory of discrete state, continuous time Markov processes. For point or lumped systems, Master equations of the forward and backward type can be derived for the probability of finding a neutron population of a certain size at a certain time (Bell, 1963, 1965; Williams, 1974; Pazsit and Pal, 2008; Prinja and Souto, 2009; Prinja, 2012). Both approaches yield systems of differential-difference equations for the neutron number Probability Density Function (PDF), with one distinction being that the backward Master equation is nonlinear in the PDF while the forward equation is linear. A key advantage of the backward formulation is that it is not necessary to first obtain the complete neutron number distribution from which to then extract the extinction or survival probabilities, as is the case with the forward approach. Starting with the backward Master equation written in terms of the generating function, explicit and

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http://dx.doi.org/10.1016/j.anucene.2015.11.001
0306-4549/

closed, albeit nonlinear, differential equations for the extinction and survival probabilities can be directly written down (Bell, 1965; Pazsit and Pal, 2008; Prinja, 2012). Moreover, this can be done for both the lumped case and unlumped case where the neutron phase space dependence is also included. The backward formulation therefore allows accurate numerical calculation of these probabilities under quite general conditions while also enabling analytical solutions to be constructed when the physical model can be simplified.

What appears not to have been addressed in the literature is a systematic quantification of the effects of uncertainty in the physical parameters on the extinction and survival probabilities. The principal parameters with respect to which uncertainty analysis would contribute to a better appreciation of the impact of growth and termination of chains are nuclear data – cross sections, fission neutron multiplicities, and the strength of the intrinsic neutron source (e.g., spontaneous fission rate) – and, in a lumped model, gross parameters such as the neutron lifetime as well as the system reactivity. The relatively small number of compilations of multiplicity data for fissile materials in the open literature confirm the large uncertainties in the different measurements reported (Diven et al., 1956; Zucker and Holden, 1986; Orndoffl, 1957). On the other hand, considerable effort has been devoted over the years to reducing cross section data uncertainty for the important fissile materials. However, the intrinsic source strength is generally not known with good accuracy (Radkowsky, 1964) and the uncertainty in the neutron lifetime is potentially large as effects of physical geometry, material heterogeneity, and energy dependence are collapsed and encapsulated in a single parameter for use in a one speed point model. Moreover, depending on the application, the system reactivity may also be subject to uncertainty.

In this paper we use a lumped backward model to carry out a detailed numerical investigation of the effect of physical parameter uncertainty on the time-dependent single neutron chain survival probability and the time-dependent extinction probability when an intrinsic random source is present. Specifically, uncertainty is introduced in the factorial moments of the fission neutron multiplicity distribution, the source strength and the neutron lifetime, and all parameters are assumed to be independent random variables each uniformly distributed about their respective reference values. Strictly speaking, the uncertainty should be introduced directly into the fission neutron multiplicities and propagated into the factorial moments but the constraint that the multiplicity distribution be normalized correlates the multiplicities and significantly complicates the uncertainty analysis. Although stochastic UQ methods of the type considered here can be readily extended to accommodate correlated, Gaussian distributed input variables, more advanced techniques are necessary to represent correlated non-Gaussian distributed input variables (Park et al., 2015). For this reason we have, in this preliminary investigation, incorporated uncertainty directly into the factorial moments, source strength and neutron lifetime and defer a more rigorous representation of uncertainty in the multiplicities to a more comprehensive future investigation. The multiplication factor or k-eigenvalue is generally considered to be an accurately known parameter for use in lumped systems, unlike the intrinsic source and neutron lifetime, so it is not treated as an uncertain variable this work. We emphasize that this does not represent a limitation of the methodology as it simply adds an extra independent random variable, albeit at increased computational cost.

We further emphasize that one goal of this investigation is to consider the effect of uncertainty due to the lumping of distributed systems, which constitutes another layer of uncertainty over the uncertainty in underlying cross sections and numerical approximation schemes. This arises because in the derivation of any value for the lumped system an assumption regarding the neutron flux in terms of space, energy and angle must be made in order to perform the appropriate averaging. However, particularly when the neutron population is very low (as is the case in the systems studied in this paper) the neutron flux is inherently stochastic in this regard which introduces a further uncertainty beyond that of the uncertainty of the neutronics data of the medium in which the neutrons exist. A rigorous treatment of uncertainty propagation in the neutron chain probabilities of interest here, one where uncertainty can be introduced in the fundamental measured parameters (cross sections, multiplicities), must be based on an unlumped backward Master equation formulation that accommodates space, energy and angle dependence and, although merited, such a study would be computationally very demanding and beyond the scope of the present investigation. We hope to report on a more thorough investigation along these lines at a later date.

The polynomial chaos method is used to express the output uncertainty in a spectral expansion and stochastic collocation applied to obtain and solve uncoupled equations for the deterministic expansion coefficients. This representation gives a full statistical characterization of the uncertainty in the survival and extinction probabilities of interest here from which statistical moments as well as PDFs are extracted in post processing. Finally, a global sensitivity analysis is performed using High Dimensional Model Representation (HDMR) which yields the relative contribution of each random variable to the total variance. We emphasize that these results are not subject to the restriction of linear sensitivity theory and hence provide a reliable quantification of the sensitivity to each input parameter.

The scope of the paper is as follows. In the next section we present the backward model for the survival and extinction probabilities, provide the reference data, and give a closed form analytical solution for a special case that is useful for benchmarking the numerical solution method used. Numerical solutions for baseline or reference parameters are presented and discussed in the following section. A general framework for conducting uncertainty analysis is then presented along with analytical solutions for the PDFs of the unknowns in a special case. The generalized polynomial chaos method for uncertainty quantification is introduced in the next section and detailed numerical results and analysis from the implementation of this method using non-intrusive sparse grid quadrature methods and global sensitivity analysis are presented. We present some concluding remarks in the final section.

2. Backward equations for the extinction/survival probability

The backward equations for the single chain survival probability $P(t)$ and the extinction probability for random source sponsored chains $P_E(t)$ are well known (Bell, 1965; Pazsit and Pal, 2008; Prinja, 2012) and may be expressed as:

$$\frac{\partial P(t)}{\partial t} = \left(\frac{k_{\text{eff}}-1}{\tau}\right)P(t) - \frac{p_f}{\tau}\sum_{i=2}^{\chi_{max,f}}(-1)^i\frac{\chi_{i,f}}{i!}[P(t)]^i, \quad P(0)=1, \tag{1}$$

$$\frac{\partial P_E(t)}{\partial t} = S_0\left[\sum_{i=1}^{\chi_{max,s}}(-1)^i\frac{\chi_{i,s}}{i!}P^i(t)\right]P_E(t), \quad P_E(0)=1. \tag{2}$$

In the above, τ is the neutron lifetime, p_f is the probability of fission, k_{eff} is the system multiplication factor, S_0 the intrinsic source strength, $\chi_{i,f}$ and $\chi_{i,s}$ are the factorial moments of the neutron multiplicity distribution for fission and the source respectively and $\chi_{max,f}$ and $\chi_{max,s}$ define where the relevant sums are truncated. These values are not, in general, required to be identical but, for the systems we describe in this paper, we assume the source and fission have the same neutron multiplicity distribution (i.e., the