Radiation Physics and Chemistry ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

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

Neutron transport simulation (selected topics)

P. Vaz

Instituto Tecnológico e Nuclear, Estrada Nacional 10, P-2686-953 Sacavém, Portugal

ARTICLE INFO

Keywords:
Neutron
Transport
Simulation
Deterministic
Monte Carlo
Cross-section

ABSTRACT

Neutron transport simulation is usually performed for criticality, power distribution, activation, scattering, dosimetry and shielding problems, among others. During the last fifteen years, innovative technological applications have been proposed (Accelerator Driven Systems, Energy Amplifiers, Spallation Neutron Sources, etc.), involving the utilization of intermediate energies (hundreds of MeV) and high-intensity (tens of mA) proton accelerators impinging in targets of high Z elements. Additionally, the use of protons, neutrons and light ions for medical applications (hadrontherapy) impose requirements on neutron dosimetry-related quantities (such as kerma factors) for biologically relevant materials, in the energy range starting at several tens of MeV. Shielding and activation related problems associated to the operation of high-energy proton accelerators, emerging space-related applications and aircrew dosimetry-related topics are also fields of intense activity requiring as accurate as possible medium- and high-energy neutron (and other hadrons) transport simulation. These applications impose specific requirements on cross-section data for structural materials, targets, actinides and biologically relevant materials.

Emerging nuclear energy systems and next generation nuclear reactors also impose requirements on accurate neutron transport calculations and on cross-section data needs for structural materials, coolants and nuclear fuel materials, aiming at improved safety and detailed thermal-hydraulics and radiation damage studies.

In this review paper, the state-of-the-art in the computational tools and methodologies available to perform neutron transport simulation is presented. Proton- and neutron-induced cross-section data needs and requirements are discussed. Hot topics are pinpointed, prospective views are provided and future trends identified.

1. Introduction

Accurate simulation of particle transport is closely related to the existence of cross-section data for a required range of energies and for the different types of particles, interactions and materials considered.

Neutron transport simulation has been historically performed mainly for the modeling of criticality, power distribution, activation, scattering, dosimetry and shielding problems, for neutron applications in the energy range below 20 MeV. However, in recent years, it has become necessary to have a description of the (n, xn) reactions and (n, charged) reactions among others in addition to the main types of neutron interactions (elastic and inelastic scattering, neutron capture, neutron-induced fission). This is due to a number of new applications involving the radiation field and particles with energies higher them 20 MeV as well as the need to undertake studies from the point if view of radiological protection, and the dosimetry of high-energy particles and radiations, namely neutrons. In the high-energy regime, reaction kinematics dramatically changes the cross-section for the production of multiple neutral and charged particles.

The need to improve the knowledge of proton- and neutron-induced interaction mechanisms arose from the fact that many innovative applications involved the production of intense neutron fluxes by protons impinging on a thick target of a heavy element (mercury, lead, bismuth, tungsten, uranium, etc.) and triggering a cascade of nuclear reactions, often referred to as *spallation reactions*, of the protons themselves as well as of the neutrons, and other hadrons (e.g., pions), nuclear fragments (alpha-particles, tritium, deuterium) and photons produced during the successive stages of the cascade.

Also contributing to the increasing number of high-energy proton accelerators for fundamental research purposes (High-Energy Physics experiments, Spallation Neutron Sources, etc.) was the different applications from the Nuclear Technology (Acceleration Driven Systems for the transmutation of nuclear waste, Energy Amplifier Systems for the production of energy, in Medicine for hadrontherapy) for the purposes of radiation protection, neutron dosimetry, shielding design and activation of components and

E-mail address: pedrovaz@itn.pt

0969-806X/$ - see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.radphyschem.2009.04.022

materials and for the assessment of the radiation damage caused to structural materials and the potential modification of their thermal and mechanical properties, leading to the effective improvement of the description and modeling of proton- and neutron-induced reactions.

The growing degree of awareness of the potential exposure of individuals to high-energy cosmic radiations, a major component being in aircraft dosimetry and space dosimetry due to high-energy and high-LET neutrons, also dictated the need to understand and improve the modeling of high-energy hadronic interactions.

Medium- and high-energy neutrons impose stringent and specific shielding requirements. Deep penetration of neutrons and the calculation of fluxes and doses deep inside the materials used for shielding are typical examples of computations where computing power is not always available and the use of variance reduction techniques is mandatory.

In recent years, several solutions for the design of the next generation nuclear reactors have been proposed. These nuclear reactors would operate in non-conventional regime (fast neutrons, higher temperatures and innovative fuels) and would impose requirements on accurate 3-D and time-dependent neutron transport calculations and on cross-section data needs for structural materials, coolants and fuels, aiming at improved safety and detailed thermal-hydraulics and radiation damage studies.

For the design, project and deployment of equipments and infrastructures involving the operation and manipulation of these proton beams and neutron fluxes, the uncertainty analysis studies performed clearly showed that the high uncertainty (often several tens of percent) of the existing cross-section data and on the predictive power of the theoretical models, would affect the confidence bounds of predictions meaning the application of larger safety margins in the dimensioning of shielding elements, the safety assessment and therefore the construction and operation costs of the system.

In the present paper, the specific issues and characteristics of the neutron interactions with matter will be firstly described through the analysis of the behavior of the cross-sections of selected nuclides. Afterwards, a description of the innovative and emerging applications requiring accurate neutron transport simulation and imposing specific data needs will be provided. Finally, the state-of-the-art deterministic and Monte Carlo computational methods and techniques currently available to perform the transport of neutrons and other hadrons will be reviewed and discussed; the emerging importance of hybrid methods will be presented; associated cross-section data issues will be pinpointed.

2. Neutron interactions with matter

2.1. Neutron cross-section data—specific issues

In order to accurately perform neutron transport simulation, the knowledge, for each nuclide, of the variation with energy of the competing interaction mechanisms (neutron elastic and inelastic scattering, neutron radiative capture, neutron-induced fission, etc.), is mandatory in order to assess the physics properties of the problem being studied and to accurately model its behavior.

One of the striking characteristics of the neutron interactions with matter is the relatively "poor predictive" power in cross-section behavior modeling as a function of the neutron energy, for different elements and for different nuclides of the same element.

Another feature of neutron interactions with matter is the very wide energy range over which neutrons must be transported, often spanning more than eleven energy decades, from the hundreds of MeV (or higher) down to the meV range (or lower). Knowledge of the cross-sections over the whole energy range concerned is required.

The resonant behavior is another specific characteristic of the neutron cross-section as a function of energy. The high number of resolved resonances in the energy range below a few keV and the accurate knowledge of the characteristics (peak energy, widths, etc.) of each resonance in the cross-section data libraries is an outstanding demonstration of the huge amount of experimental data extensively measured during the last decades. These characteristics and features of the cross-section for neutron-induced processes are displayed in Fig. 1.

While cross-section data exists below 20 MeV in the evaluated cross-section data libraries for a very representative set of nuclides, the situation is very (and for some nuclides dramatically) different in the energy range above 20 MeV. As shown below, a number of emerging and technological innovative applications have been proposed during the last fifteen years. Some of these are currently in the detailed design phase, while others have already been engineered and implemented. The majority of such systems involve the manipulation of unprecedented high neutron fluxes and the consideration of neutron spectra above 20 MeV, or even as high as a few GeV. The acquisition of the neutron interaction cross-sections in this very high-energy range became therefore an issue of major concern, in view of the lack of data for these energy ranges for a number of structural materials of relevance for many technological applications as well as for the biologically relevant materials, used in radiation protection and dosimetry issues.

In addition, for a representative subset of nuclides, present in the evaluated data libraries, the cross-section data showed significant discrepancies between different evaluations namely for actinides and structural materials.

A major effort was therefore undertaken during the last decade on an international scale, in order to encourage the experimental measurements for data above 20 MeV up to a few hundreds of MeV and/or compilation and evaluation of existing data sets. These data were made available through the major cross-section data libraries currently in use.

2.2. Modeling issues and sensitivity and uncertainty analysis

Data evaluation efforts are closely related to the utilization of theoretical models, the predictive power of which has to be assessed and validated.

The predictive power of theoretical models can be determined by its validation against experimental data. Additionally, benchmark exercises can be conducted in order to inter-compare the behavior of different models and their predictions. The quantities of interest are the integral cross-sections as well as the single- or double-differential cross-sections as a function of variables such as energy, angle and multiplicity of particles produced, amongst others.

The use of invalidated theoretical models, or those not benchmarked against experimental data became mandatory in situations where no or insufficient experimental data existed.

However, theoretical models often rely on "tuning" parameters used to adjust their predictions to the available experimental data; agreement between models and data can widely vary from one energy range to another; the predictions for the differential cross-sections (as a function of the energy, of the angle, etc.) can be substantially different from one model to another; and the differential cross-section for exclusive or inclusive measurements can also deviate significantly from the experimental data measurements and from one model to another.

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

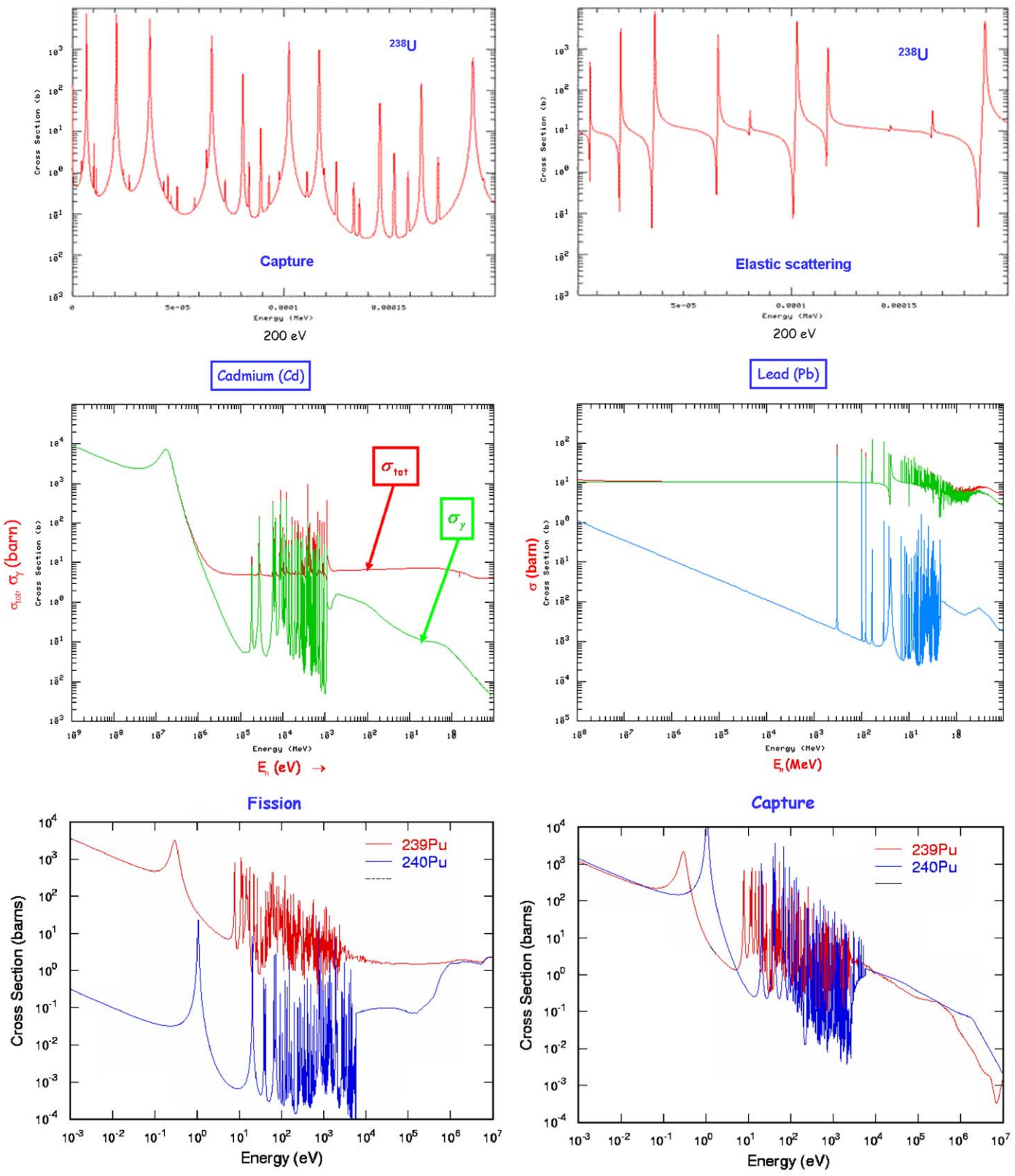


Fig. 1. Examples of the quick variation with energy of the neutron cross-sections and of the resonant behavior of the cross-sections (top), of the completely different behavior of the cross-sections and types of interactions for different elements (middle) and of the variation of the behavior of the interaction mechanisms for isotopes of the same element (bottom).

Computer codes that perform neutron (as well as other hadrons) transport normally rely on a set of theoretical models and adjustable parameters that can be activated by the user.

The utilization of theoretical models became of paramount importance in recent years for the modeling and simulation of emerging and innovative applications involving the utilization of

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

high-energy (above 20 MeV) radiation fields, as described in the following section. Due to the scarcity of the experimental data available for some of the relevant materials in this energy range and the need to accurately describe the proton- and neutron-induced reactions and the associated spallation processes, a variety of theoretical physics models have been developed and implemented in Monte Carlo computer codes. These models attempt to describe the various stages of development of the intranuclear and internuclear cascades. An extensive review of such models can be found in Maschnik et al. (2000).

However, relatively few studies have been performed for the different applications on the sensitivity of the simulation results (namely calculations of fluxes and doses) to the uncertainty on the cross-section data used during the transport of neutrons and other hadrons. Recent parametric studies indicate that the uncertainty of the simulated results due to the uncertainty of the input cross-section data used can range from a few percent up to several tens of percent, indicating, as could be expected, that the uncertainty of the different types of interactions affects the computed quantities differently.

3. Emerging and innovative applications

3.1. Neutrons and technology

As pointed out in Thomas (2004) there is an increasing trend to an increase of exposure of individuals to high-LET radiations, due to technological developments. The same author also points out that dosimetry of high-energy radiation is an area where clarification is needed in the ICRP recommendations. Additionally, a revision of the parametrization of the radiation weighting factor as a function of the energy has been proposed by the ICRP in its recent publication (Recommendation of the International Commission on Radiological Protection, 2005).

A number of technological applications implementing innovative nuclear systems have been proposed in recent years; some of them are briefly reviewed in the following sections. Aircrew dosimetry and space-applications related issues also contributed to the need to perform sound studies on cosmic radiation as explained in the following sections.

3.2. Accelerator driven systems (ADS) and energy amplifiers (EA)

Accelerator driven systems (Vanneri et al., 1993; Rubbia et al., 2001; Giraud et al., 2005a) and energy amplifiers (Rubbia et al., 1993, 1995) are hybrid systems consisting of a sub-critical reactor coupled to a high-intensity (beam current in the several mA range) and proton accelerator impinging on a high-density target (liquid lead, lead-bismuth eutectic, etc.). The spallation reactions triggered by the "high-energy" protons (in the 600–1000 MeV range) in the target result in very high (of the order of 10^{15} neutrons/cm/s) and fast (neutron energies above several hundreds of keV) neutron fluxes used to induced capture and fission reactions in the surrounding core consisting of assemblies that contain fuel elements enriched in actinides. ADS have emerged in recent years as a promising solution to the long standing problems of transmutation of the high-level and highly radiotoxic wastes (plutonium, americium and curium isotopes as well as some of the long-lived fission fragments) in the spent fuel of nuclear power reactors.

The problems arising in the projected ADS systems are typically associated with the evaluation of the neutron fluxes in the target and surrounding core and the associated neutron transport throughout the system, for assessing criticality and determining the sub-criticality level, for the design of the shielding system and associated radiological protection issues, for determining the spatial power distribution in the target and surrounding system components (coolant, fuel assemblies and the fuel itself) for thermal-hydraulic calculations associated with the study of the transient and steady state behavior of the system of relevance for its nuclear safety assessment.

Fig. 2, extracted from Giraud et al. (2005b), displays results from Monte Carlo computations of the spatial mapping of the neutron fluxes and energy deposition in the target of an ADS system, with a proton beam of intensity of 600 MeV incident in a liquid lead-bismuth eutectic target.

The high-energy and high-intensity of the proton accelerator impose stringent requirements on the design of the beam line, from the radiation protection and shielding point view.

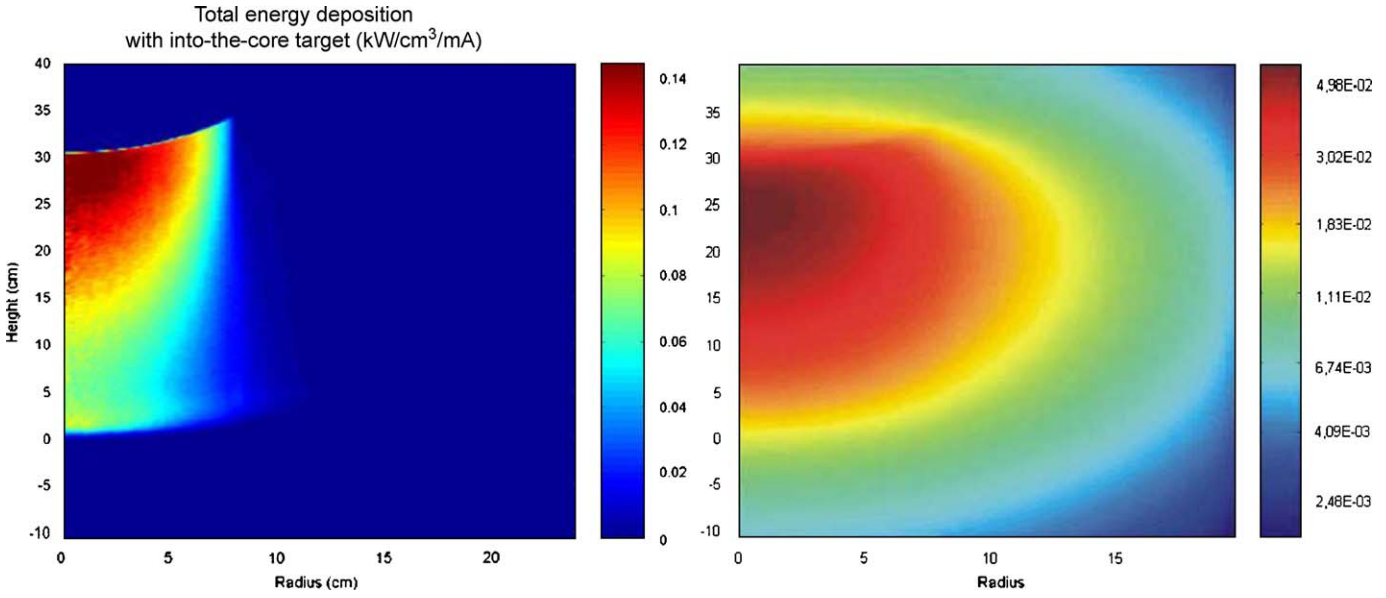


Fig. 2. Spatial mapping of the energy deposition (left, in kW/cm^3/mA) and the neutron flux (right, n/cm^2/incident proton) in the target of an ADS system. The proton beam impinges vertically and has an elliptic distribution of radius 8 cm.

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

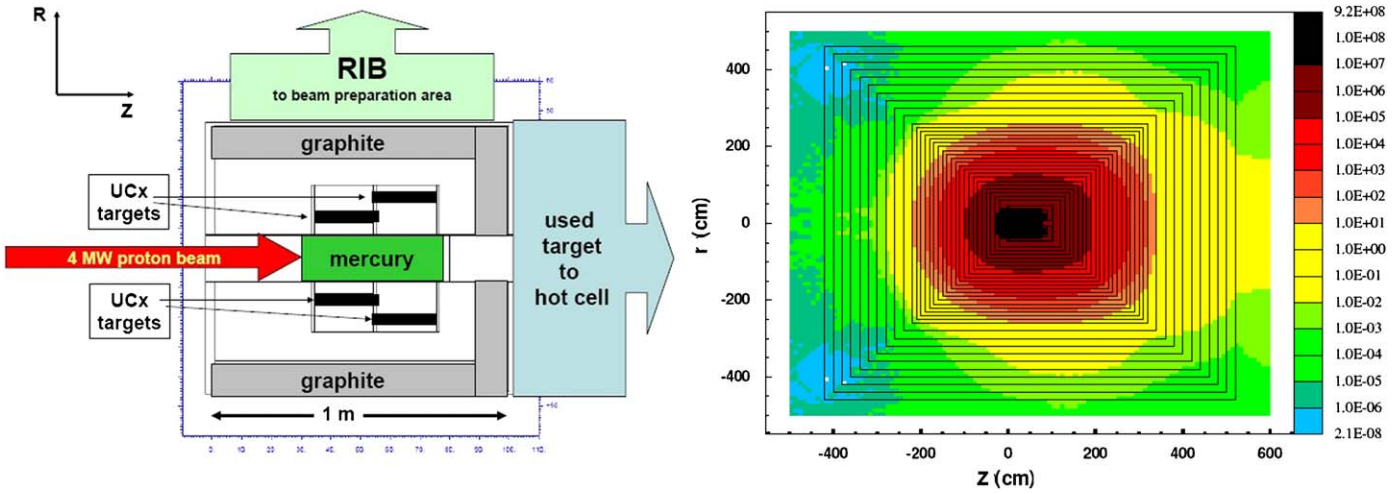


Fig. 3. Target description of the EURISOL facility (left) and computed dose distribution in the surrounding 2 m thick iron shielding (right)

3.3. *High-power (multi-megawatt) targets*

Today, these facilities involve two main categories of projects: multi-megawatt targets for the production of radioactive ion beams (e.g., the EURISOL project; Vervier et al., 2003), and spallation neutron sources (e.g., the Spallation Neutron Source in the USA; Spallation Neutron Source, 2000—but also different projects in Europe and Japan in recent years). Both categories of projects have in common the high-power delivered by a proton beam of energy from the hundreds of MeV up to a few GeV range.

The target materials considered are normally mercury, tungsten, tantalum and in some cases uranium, with proton energies up to a few GeV being considered in the design studies.

Fig. 3 extracted from Felcini et al. (2006) provides information about the multi-megawatt target of the EURISOL facility currently in and advanced design phase, and the Monte Carlo simulation of the computed dose in the target and surrounding shielding.

3.4. *Aircrew and space dosimetry*

The intense campaign of measurements carried out in commercial airplanes on different routes and at different latitudes, has made possible the assessment of dose rates in the range 6–10 μSv/h for several flights connecting major cities worldwide. These measurements contributed to increasing the degree of awareness of the fact that the annual exposure of aircrews can be estimated in the few mSv range, making them one of the professional categories more exposed to ionizing radiations. As shown in Reitz (1993) and Schraube (2003), at typical altitudes of commercial long-distance flights (10–11 km), neutrons are amongst the main contributors to the total dose rates arising from exposure to cosmic radiation.

Additionally, in recent years different studies and observations of solar particle events (SPE) due to the solar activity and the assessment of the doses resulting from the exposure of crews of space flights to radiation bursts from galactic cosmic rays (GCR) contributed to transform neutron (and other high-energy particles) dosimetry in a top priority issue with the need to compute, via Monte Carlo simulations, the fluence to effective dose and fluence to ambient dose equivalent conversion coefficients in energy ranges up to several TeV (Pelliccioni, 2000). Fig. 4 from Sakamoto et al. (2006) displays the significant increase at very high energies of the fluence to effective dose conversion coefficients for neutrons that are obtained for energies above 20 MeV by Monte Carlo simulation of neutron transport.

3.5. *Radiation protection and neutron dosimetry issues*

The new parameterization of the neutron radiation weighting factor as a function of energy proposed in Recommendation of the International Commission on Radiological Protection (2005) and the gradual improvement of the scientific knowledge of the biologic effects of radiations including those due to exposure of neutrons paves the way for developments in the simulation of neutron transport for biological purposes. Fig. 5 from Recommendation of the International Commission on Radiological Protection (2005) displays the time evolution of the neutron radiation weighting factors recommended by the ICRP, as a function of time.

The need to determine the kerma factors and other neutron dosimetry-related quantities in the energy range above 20 MeV for biologically relevant materials constituents of tissue and bones has been pinpointed in Chadwick et al. (1997). Due to the difficulty in carrying out experiments to make the determination of these quantities possible, as before, the computational determination of such quantities using Monte Carlo methods to model the neutron transport and interactions is a natural solution for the determination of such quantities.

Monte Carlo simulations of neutron transport inside the human body for different incidence geometries of the radiation field have also been conducted in recent years in order to determine the tissue weighting factors, whose knowledge is mandatory for the assessment of the effective dose.

3.6. *Nuclear energy "renaissance"?—generation III+ and generation IV nuclear reactors*

The recent renewed interest in nuclear energy since a few years, concentrates on two types of reactor concepts that can be broadly categorized as GEN III+ (evolutionary concept, to be deployed during the next few decades) and GEN IV (new family of reactors, to be deployed after that).

It is generally considered by the experts that both categories of reactors will imply considerable neutronics studies in order to improve their safety (decreasing the probability of severe-core damage accidents down to 10^{-6}/year amongst other criteria) and

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

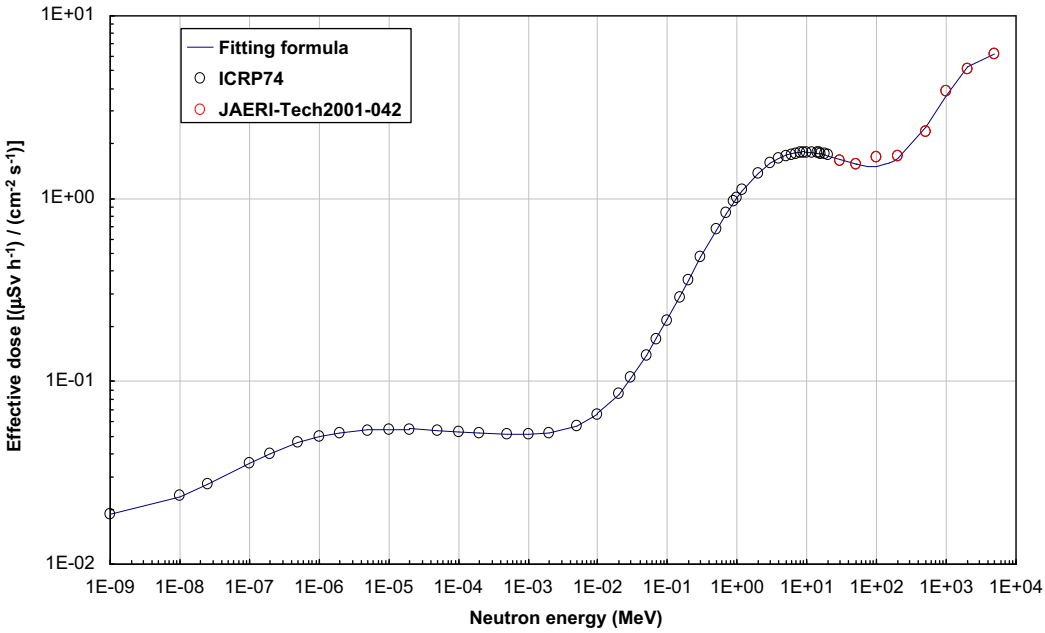


Fig. 4. Fluence to effective dose conversion coefficients for neutrons of energies up to 5 GeV. The eight rightmost coefficients (for energies greater than 20 MeV) are from Sakamoto et al. (2006).

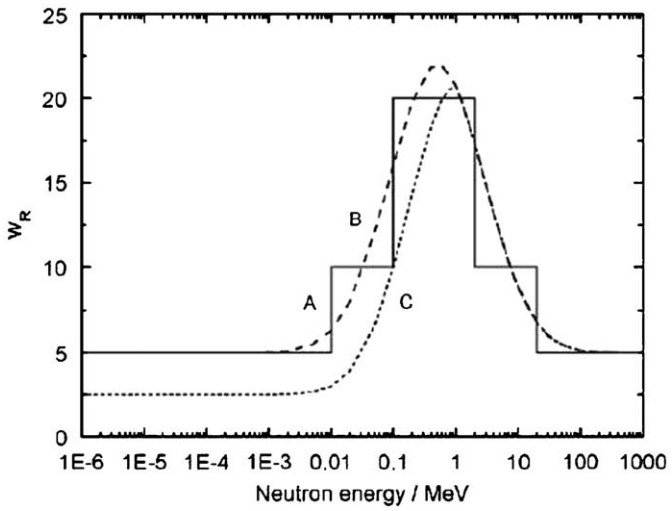


Fig. 5. Neutron radiation weighting factors as a function of energy: situation before 1991 (histogram A), parameterization from ICRP-60 recommendation (curve B) and the latest ICRP recommendation proposed in 2005 (curve C)

to accommodate by proper core design, higher fuel burn-ups (exceeding 50 MWd/kg), higher power (up to 1600 GWe in the GEN III+ reactors), improved efficiency and overall economics, with minimization of the spent fuel volumes and radiotoxicity to be sent to the geological repositories and complementary disposal solutions.

The study of safety sequences and of the thermal-hydraulics behavior (both in transient and steady state mode) of these reactors are two of the issues to be addressed by proper simulation of these nuclear systems.

Additionally, some of the GEN IV reactor concepts address various innovative issues in reactor physics, such as different coolants (e.g., sodium-, gas- or liquid-metal cooling) and high temperature of the fuels (HTR).

It is the view of experts that the renaissance of nuclear energy will have to consider fast reactors (harder neutron energy spectrum enriched in the MeV region compared to the traditional light water reactors), with advanced fuel cycles considering reprocessing, recycling and non-standard fuels including higher actinides (plutonium, americium, curium) enriched fuels in the burner mode.

This whole set of characteristics needs complex neutronics calculations with special design of the reactor cores and fuel assemblies considered, through a detailed geometrical description of the system and a highly granular spatial determination of the fluxes and doses.

Calculations of the radiation damage in the materials subject to the intense fast neutron fluxes will also require a detailed simulation of the systems in order to assess potential changes of the thermal and mechanical properties of the fuel claddings, the fuel itself during transient sequences and of the other structural materials.

It goes without saying that shielding studies and radiological protection related studies have to be further pursued in view of the fast neutron fluxes and improved safety requirements inherent to this new generation of reactors.

3.7. Hadrontherapy

The shielding of proton and light ion therapy facilities is dictated by the behavior of the neutrons with energies up to almost the beam energy. The several meters concrete and/or several tens of centimeters of iron and/or several meters of ground surrounding the facilities does certainly influence the construction costs (due to the volumes of shielding materials to be used) of such facilities.

3.8. Security applications

Applications using the neutron radiography technique or exploiting the neutron scattering characteristics in order to

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

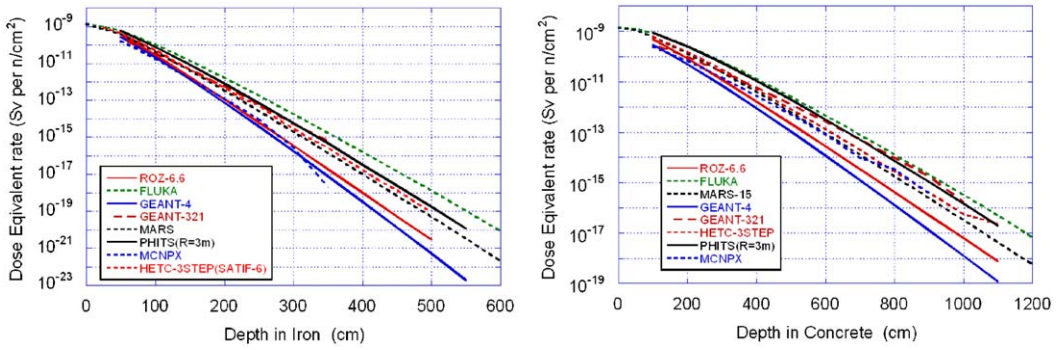


Fig. 6. Neutron dose attenuation for 1 GeV neutron impinging on iron and concrete slabs, computed by different Monte Carlo codes.

increase sensitivity in the detection of explosives and of illegal traffic of radioactive substances can be foreseen in the medium term future. One of the drawbacks of the utilization of neutrons is related to the radiological protection of professionals and members of the public. Another drawback concerns to the logistic aspects associated with the dimensions of such facilities and their deployment in public places.

3.9. Deep penetration problems and neutron attenuation

Shielding of medium- and high-energy (proton) accelerators imposes stringent requirements on the cross-section data and modeling for both proton- and neutron-induced reactions. High-energy neutrons are highly penetrating and different values of the neutron attenuation length as a function of energy can be obtained using different computer programs.

Accurate neutron transport requires experimental and evaluated data (whenever available) or reliable predictions from sound theoretical models. As shown in Fig. 6 extracted from Hirayama (in press), several computational benchmark exercises indicate indeed that at several meters deep inside concrete and iron shields, the computed (via Monte Carlo simulation) neutron fluxes and doses vary widely, sometimes by factors ranging between 10 and 100. This is mostly due to the lack of experimental information on the attenuation of high-energy neutrons (in the hundreds of MeV range) and to the lack of data for those energy ranges and for the shielding materials. In this context, experiments on attenuation and deep penetration of neutrons in shields are required, as identified in Hirayama (in press).

The computation of the doses behind the shielding elements becomes a major issue in accelerator shielding, with repercussion both on the radiological protection and also on the economics (construction and operation costs) of the facilities requiring the operation of medium- and high-energy proton accelerators.

4. Neutron transport simulation

The ultimate goal (the vision) in neutron transport simulation consists in performing detailed 3-dimensional, time-dependent, neutral- and charged-particle transport calculations *efficiently* and *accurately*.

Historically, neutron transport simulation was first attempted successfully by deterministic methods, solving numerically the Boltzmann neutron transport equation in its integro-differential or integral form, presented in the following. Considering the angular and spatial discretization, and the energy grouping described in the sequence and inherent to the methodology adopted for solving the Boltzmann transport equation, it turns out that large hardware (computer memory) is required in order to achieve a reasonable spatial discretization of the system geometry and to accurately describe the physics processes and interactions taking place.

However, in recent years, the emerging and innovative technological applications requiring the consideration of higher than 20 MeV neutrons did imply a re-analysis of the Boltzmann transport equation in order to incorporate reaction channels (such as (n, xn)) in the balance of neutrons.

The advent of powerful processors and computer architectures since the early 1990's made possible the increasingly important utilization of Monte Carlo simulation programs to model complex systems, both from the point of view of the physics (type of particles and interactions, energy ranges, etc.) and from the point of view of a detailed geometrical description. However, it turns out that due to the intrinsic methodology of the Monte Carlo simulations, systems with a highly complex geometry and physics and implying very high fluxes and doses (thick shields required) sometimes require prohibitive computation times. As seen in the sequence, a number of variance reduction techniques have been implemented in the majority of the state-of-the-art Monte Carlo computational tools, aiming at reducing the uncertainty of the computed results by means of using weighting techniques and importance criteria, among others, and giving rise to non-analog Monte Carlo techniques.

In recent years, a number of authors have developed computational tools that implement a variety of hybrid methods and try to solve numerical problems associated with the convergence of the solution and to implement more effective differencing schemes (for the derivatives) and to prevent problems associated with the sometimes very rapid spatial variation of the flux in the systems being simulated. Such methods are called hybrid and in some cases use the adjoint solution of the Boltzmann transport equation coupled with the Monte Carlo simulation techniques. In the sequence several methods are described and analysed. An excellent review is provided in Haghighat (2004).

4.1. Deterministic methods

Extensive formulations of the deterministic methods applied to neutron transport calculations can be found in Lewis and Miller (1993) and O'Dell and Alcouffe (1987), among many others. The Boltzmann neutron transport equation establishes in its general integro-differential time-dependent form, the neutron balance (neutron production minus neutron losses) in the 7-dimensional phase space element $d^3rd^2\Omega dEdt$, at point r, within the angular cone $d^2\Omega$ about direction Ω (unit vector), with

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

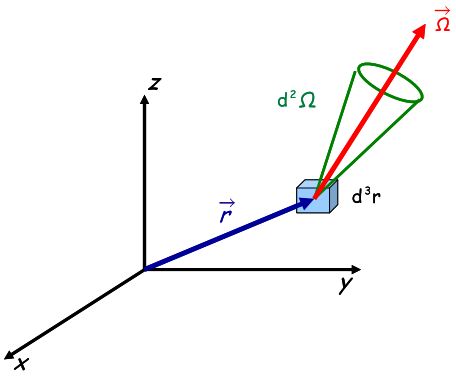


Fig. 7. Spatial and angular coordinates considered for writing the Boltzmann neutron transport equation that establishes the neutron balance inside the elemental volume d^3r at position r and within the angular cone $d^2\Omega$ around direction Ω.

energy in the interval dE about E and at time dt about t, as shown in Fig. 7.

The linear Boltzmann transport equation establishes that the time variation of the neutron density $\partial n/\partial t$ inside the phase space element $d^3r d^2\Omega dE$ can be written as

$$\underbrace{\frac{1}{v}\frac{\partial}{\partial t}\phi(\vec{r},E,\vec{\Omega},t)}_{\partial n/\partial t} = \underbrace{-\vec{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega},t)}_{\text{“streaming”}} \underbrace{-\sum_{tot}(\vec{r},E)\phi(\vec{r},E,\vec{\Omega},t)}_{\text{Absorption+scattering}}$$
$$+\underbrace{\int_0^\infty\int_{4\pi}\sum_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}',t)\,d^2\Omega'\,dE'}_{\text{scattering}}$$
$$+\underbrace{\frac{1}{4\pi}\chi(\vec{r},E)\int_0^\infty\int_{4\pi}\nu(\vec{r},E')\sum_f(\vec{r},E')\phi(\vec{r},E',\vec{\Omega}',t)\,d^2\Omega'\,dE'}_{\text{fission}}$$
$$+\underbrace{\sum_{x=2}^{\infty}\int_0^\infty\int_{4\pi}(x-1)\cdot\sum_{n,xn}(r,E',\Omega',t)\phi(\vec{r},E',\vec{\Omega}',t)\,d^2\Omega'\,dE'}_{n,xn}$$
$$+\underbrace{S_{ext}(\vec{r},E,\vec{\Omega},t)}_{\text{external source}}$$

being $\phi(r, E, \Omega, t)$ the neutron angular flux, v the neutron velocity, $\sum_{tot}$ the collision (absorption plus scattering) macroscopic cross-section, $\sum_s$ the macroscopic neutron scattering cross-section, $\sum_{fiss}$ the macroscopic neutron fission cross-section, $\Sigma_{n,xn}$ the macroscopic cross-section for the (n, xn) process, ν the number of neutrons generated by fission and χ the energy spectrum of the fission neutrons. Spherical harmonics series and Legendre polynomial expansions are commonly used to represent the angular dependence of the scattering cross-section ($\sum_S$) and the inhomogeneous (if that's the case) external source term (S_{ext}).

The steady state (time derivative set to zero and time dependence ignored in the previous equation) can be written in a more compact format, as

$$\underbrace{\vec{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega})}_{\text{streaming}}+\underbrace{\sum_{tot}(\vec{r},E)\phi(\vec{r},E,\vec{\Omega})}_{\text{“collision”}}=\underbrace{q(\vec{r},E,\vec{\Omega})}_{\text{“source”}}$$

with the “source” term grouping the different terms (corresponding to the external source, to fission, to scattering and to (n, xn) reactions) in the previous formulation.

Amongst many other applications, the Boltzmann transport equation has been frequently used for solving the so-called eigenvalue calculation, attempting to determine the effective multiplication factor k_{eff}, the eigenvalue of the following Boltzmann equation

$$\underbrace{\vec{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega})}_{\text{“streaming”}}+\underbrace{\sum_{tot}(\vec{r},E)\phi(\vec{r},E,\vec{\Omega})}_{\text{Absorption+scattering}}$$
$$=\underbrace{\int_0^\infty\int_{4\pi}\sum_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}')\,d^2\Omega'\,dE'}_{\text{scattering}}$$
$$+\underbrace{\frac{1}{k}\frac{1}{4\pi}\chi(\vec{r},E)\int_0^\infty\int_{4\pi}\nu(\vec{r},E')\sum_f(\vec{r},E')\phi(\vec{r},E',\vec{\Omega}')\,d^2\Omega'\,dE'}_{\text{fission}}$$
$$+\underbrace{S_{ext}(\vec{r},E,\vec{\Omega})}_{\text{external source}}$$

that is used to characterize the sub-critical ($k = k_{eff} < 1$), critical ($k = k_{eff} = 1$) and supercritical ($k = k_{eff} > 1$) behavior of a multiplication system, such as the core of a nuclear reactor.

In recent years, a renewed interest in the Boltzmann equation and its numerical solution has emerged, due among other methods to the characteristics of new technological applications such as ADS, with

- its inherent high-energy neutron regime, requiring the consideration of the (n, xn) reactions terms (the cross-section is no longer negligible in the energy range above 20 MeV).
- its hybrid behavior, with a proton beam impinging in a spallation target and acting as an exterior source of neutrons feeding the multiplicative, fissile materials of the core.

The last characteristics led (Salvatores, 2002) to the definition of a new multiplication factor, k_S, the so-called “source multiplication factor”. For a sub-critical system such as the core of an ADS, the relation between k_{eff} and k_S can be determined taking into consideration the operator form of the Boltzmann equation

$$A\phi_0 = \frac{1}{k_{eff}}F\phi_0 \quad \text{(absence of external source)}$$

$$A\phi_s = F\phi_s + S_{ext} \quad \text{(with external source)}$$

Defining

$$k_S = \frac{\langle F\phi_S\rangle}{\langle F\phi_S\rangle + \langle S_{ext}\rangle}$$

with $\langle F\phi_S\rangle$ and $\langle S_{ext}\rangle$ the fission and external source terms of the Boltzmann equation integrated over $d^3r d^2\Omega dE$. The previous equation can be re-written in the same form as in the absence of external source (but differing in the meaning of the multiplication factors and the fluxes!)

$$A\phi_S = \frac{1}{k_S}F\phi_S$$

In such hybrid systems, it becomes relevant to define the importance φ^* of the neutrons produced by spallation processes in the target relative to those neutrons produced by fission in the core as

$$\varphi^* = \frac{(1-k_{eff})k_{src}}{(1-k_{src})k_{eff}} = \left(\frac{1}{k_{eff}}-1\right)\cdot\frac{\langle F\phi_s\rangle}{\langle S_{ext}\rangle}$$

4.1.1. The numerical solution of the Boltzmann equation

Except for a reduced number of cases, no analytic solution to this equation can be determined even in its simplified forms, namely in the absence of external neutron source ($S_{ext} = 0$), in non-fissile material (the fission term vanishes) and for the energy range where the contribution from the (n, xn) terms is negligible.

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

For the majority of the real applications and systems, this equation is solved numerically for the particle fluxes $\phi(r, E, \Omega, t)$, using a three-fold discretization:

- Energy discretization (multigroup formalism).
- Angular discretization (the most popular and widely used method is the commonly referred to as the S_N method).
- Spatial discretization (consisting of finite differences methods and differencing schemes of variable complexity and accuracy).

4.1.2. Energy discretization—the multigroup formalism

The multigroup formalism consists in dividing the whole energy range of interest in G energy intervals, such that

$$\Delta E_g = E_{g-1} - E_g, \quad g = 1, 2, \ldots, G$$
$$E_{\max} > E_1 > E_2 > \cdots > E_{g-1} > E_g > \cdots > E_{\min}$$

and considering for each group (and corresponding energy interval) the *flux averaged* cross-section computed as

$$\sigma_g = \frac{\int_{E_g}^{E_{g-1}} \sigma(E) \cdot \phi(E)\, dE}{\int_{E_g}^{E_{g-1}} \phi(E)\, dE}$$

is constant. Fig. 8 displays for Uranium-235, the continuous energy cross-section and a multigroup cross-section approximation.

4.1.3. Angular discretization—the S_N discrete ordinates method

The so-called S_N discrete ordinates methods consists of the selection at (r, E) of a discrete set of M directions $\{\Omega_m\}$ and associated weights $\{w_m\}$, $m = 1, \ldots, M$, in order to determine the fluxes ϕ_m:

$$\phi_m \equiv \phi(r, E, \vec{\Omega}_m),$$

with

$$\underbrace{\vec{\Omega}_m}_{\text{unit vector}} \equiv \underbrace{(\mu_m, \eta_m, \xi_m)}_{\text{direction cosines}}$$

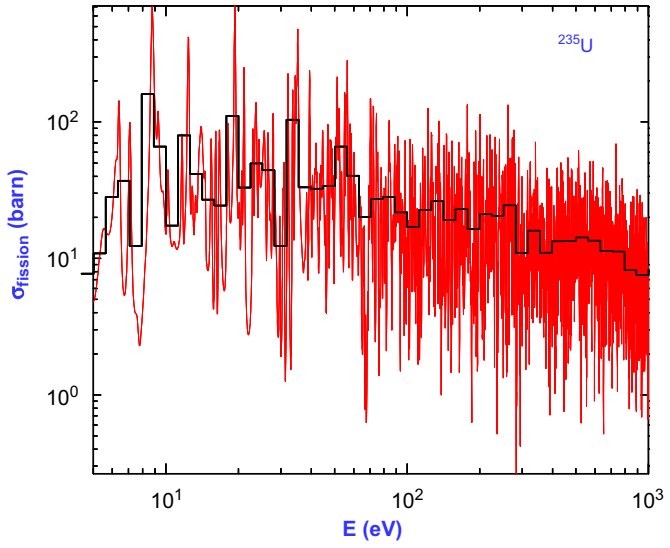


Fig. 8. Fission cross-section for Uranium-235 in the energy range from 5 to 1000 eV: continuous cross-section and a multigroup representation (histogram-like curve)

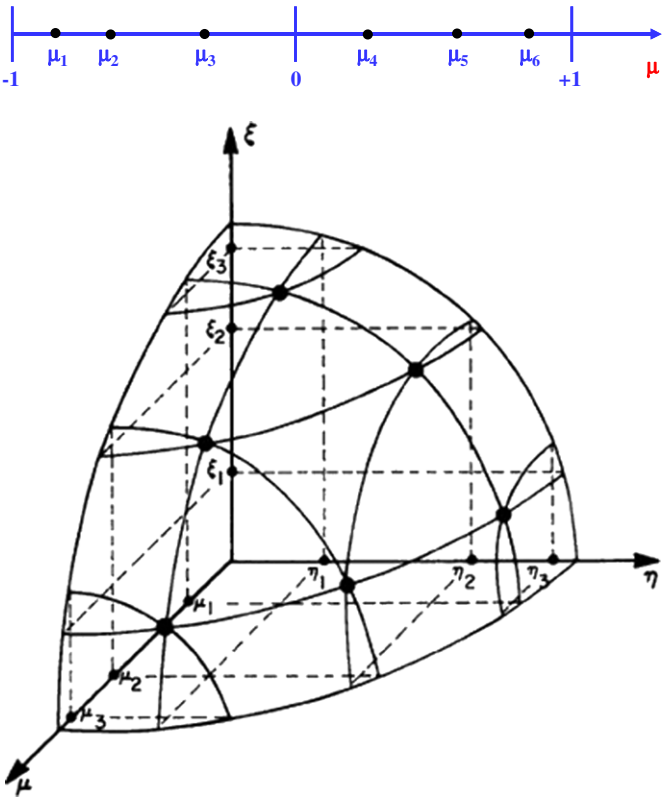


Fig. 9. S_6 angular discretization for 1- (top) and 3-dimensional (bottom) geometries.

and a set of weights

$$\sum_{m=1}^{M} w_m = 1$$

Fig. 9 depicts for 1- and 3-dimensional problems, the angular discretization for S_6 $(N = 6)$ solution.

A set of M equations is then solved as

$$\underbrace{\nabla \cdot \vec{\Omega}_m \phi(\vec{r}, E, \vec{\Omega}_m)}_{\text{streaming}} + \underbrace{\sum_{tot}(\vec{r}, E)\phi(\vec{r}, E, \vec{\Omega}_m)}_{\text{collision}} = \underbrace{q(\vec{r}, E, \vec{\Omega}_m)}_{\text{“source”}}$$

In order to determine the fluxes

$$\phi(r, E) = \int_{4\pi} \phi(\vec{r}, E, \vec{\Omega})\, d\Omega \cong \sum_{m=1}^{M} w_m \phi(\vec{r}, E, \vec{\Omega}_m) \equiv \sum_{m=1}^{M} w_m \phi_m$$

4.1.4. Spatial discretization—finite differences and other differencing schemes

A variety of differencing schemes have been developed and implemented in different deterministic codes. The underlying idea consists of superimposing on the real geometry of the system being modeled, a mesh of points and to compute the flux at each of these points. In complex differencing schemes, the mesh coarseness can be varied, according to the importance of the region being considered, finer meshes being defined for regions of rapidly varying neutron fluxes whereas coarser meshes can be defined for other regions where the flux variation is smoother.

Ideally, very fine meshes should be defined in order to obtain a very accurate description of the system and of the physical quantities being computed (namely neutron fluxes). However,

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

very fine meshes imply a huge number of space points and equations to be solved numerically, with prohibitive computer times and sometimes numerical convergence problems.

The approximate geometry of the VENUS reactor is depicted in Fig. 10 with the superimposed mesh used for the mapping of the neutron flux in the system using the deterministic code BOT3P, as reported in Orsi.

4.1.5. The adjoint equation

Most deterministic transport codes can solve the Boltzmann equation in its forward form as previously presented, as well as in its adjoint form. The adjoint solutions, namely the adjoint fluxes (ϕ^+), have the physical significance of the "importance" of particles within the systems being solved. The adjoint, time-independent transport equation form of the Boltzmann

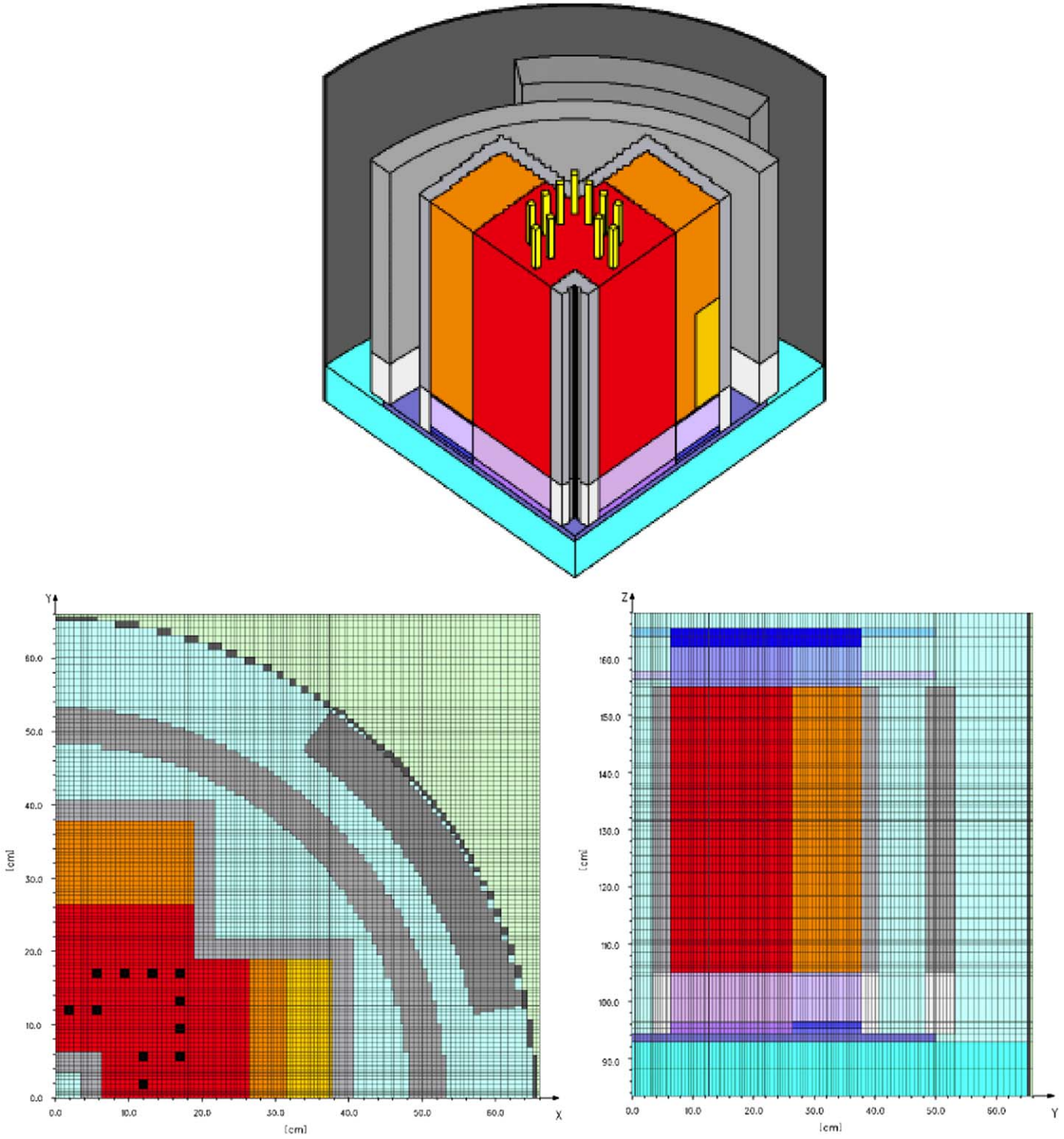


Fig. 10. Geometry of the VENUS reactor (top), and superimposed horizontal (bottom left) and vertical (bottom right) spatial meshes for a neutron flux computation using a deterministic code.

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

equation is

$$-\vec{\Omega}\cdot\nabla\phi^{+}(\vec{r},E,\vec{\Omega})+\Sigma_{tot}(\vec{r},E)\phi^{+}(\vec{r},E,\vec{\Omega})=q^{+}(\vec{r},E,\vec{\Omega})$$

with the adjoint "source" expressed as

$$q^{+}(\vec{r},E,\vec{\Omega})=S^{+}_{ext}(\vec{r},E,\vec{\Omega})+S^{+}_{F}(\vec{r},E,\vec{\Omega})+S^{+}_{S}(\vec{r},E,\vec{\Omega})$$

and the adjoint "scattering" and "fission" terms as

$$S^{+}_{S}(\vec{r},E,\vec{\Omega})=\int_{0}^{\infty}\int_{4\pi}\Sigma_{s}(\vec{r},E\rightarrow E',\vec{\Omega}\rightarrow\vec{\Omega}')\phi^{+}(\vec{r},E',\vec{\Omega}')\,d^{2}\Omega'\,dE'$$

$$S^{+}_{F}(\vec{r},E,\vec{\Omega})=\frac{1}{k}\frac{1}{4\pi}\chi(\vec{r},E)\int_{0}^{\infty}\int_{4\pi}\nu(\vec{r},E)\sum_{f}(\vec{r},E)\phi^{+}(\vec{r},E',\vec{\Omega}')\,d^{2}\Omega'\,dE'$$

The detailed discussion is outside the scope of this paper. For a lengthy and detailed derivation and discussion of the Boltzmann adjoint equation refer to the bibliography. From the computational point of view, solving the adjoint neutron transport equation represents a significant speed-up in the numerical and computational process of finding the solution of the system being described and modeled. In recent years, a number of so-called hybrid codes have been developed, combining the solution of the deterministic adjoint neutron transport equation (in order to optimize the speed of the computations) with the utilization of Monte Carlo codes (that allow the detailed description of both the geometry and the physics of the system).

4.1.6. Summary on deterministic methods

The main characteristics of the deterministic methods used to perform neutron transport simulation of physics systems are as follows:

- the formulations lead to systems of linear equations,
- requires the consideration of a computational grid (corresponding to energy, angular and spatial discretization),
- impose large computational resource requirements (the number of angular directions times the number of spatial grid points times the number of energy groups considered),
- are usually faster than Monte Carlo,
- can provide detailed 2- and 3-dimensional solutions (mapping of doses and fluxes),
- feature limited physics for higher than a few MeV neutron energy groups,
- scope for multiphysics interfacing,
- hot issues:
  - differencing schemes
  - acceleration
  - convergence

4.2. Monte Carlo methods

Conceptually, it has been shown (James, 1968; James, 1980) that Monte Carlo problems are essentially integrations. In Lux and Koblinger (1991) the authors note that "… *the idea of estimating an integral over many-dimensional space by evaluating the function at one random point in the space is far-fetched*".

As described in James (1980), Monte Carlo calculations produce a result F which is a function of random numbers ρ_i, $F\equiv F(\rho_1, \rho_2, \ldots, \rho_M)$. If the ρ_i are independent, then, as pointed out in the same reference, $F(\rho_1, \rho_2 \ldots, \rho_M)$ is an unbiased estimator of the Mth dimensional integral I, defined as

$$I=\int_{0}^{1}dx_1\int_{0}^{1}dx_2\int_{0}^{1}dx_3\ldots\int_{0}^{1}dx_M F(x_1,x_2,\ldots,x_M)$$

This integral can be solved by generating N sets of vectors of M random numbers. For each $k=1, 2, \ldots, N$, generate $(x_1^{(k)}, x_2^{(k)}, \ldots, x_M^{(k)})$ values, with $x_m^{(k)}$, $(m=1, 2, \ldots, M)$ randomly distributed in the interval $[a_m, b_m]$. Then, an estimator of the integral is obtained by computing the average of the N values of the function computed for each of the k sets of x values as

$$I\approx(b_1-a_1)(b_2-a_2)(b_3-a_3)\ldots(b_M-a_M)\frac{1}{N}\sum_{k=1}^{N}F(x_1^{(k)},x_2^{(k)},\ldots,x_M^{(k)})$$

The Central Limit Theorem and the law of the large numbers establish that as $N\rightarrow\infty$ the average value converges to the exact value of the integral.

However, if the same problem can be solved using either deterministic or Monte Carlo methods, the question of whether the Monte Carlo methods implemented in the state-of-the-art computer programs indeed solve the Boltzmann neutron transport equation seems very relevant.

4.2.1. Transition, collision and transport kernels

Conceptually, the transport of a single particle can be described as a sequence of collisions occuring at discrete spatial locations followed by the transition of the particle from one collision point to the next collision point. At collisions, the incoming particle direction and energy are changed, whereas during the transition between two consecutive collision points, the energy and direction of the particle is maintained. The integral form of the Boltzmann transport equation written in terms of the particle collision density in the 6-dimensional space $\Psi(r, \Omega, E)$ becomes

$$\underbrace{\Psi(\vec{r},E,\vec{\Omega})}_{\text{particle collision density}}=\int\left[\int\Psi(\vec{r}',E',\Omega')\cdot\underbrace{C(E',\vec{\Omega}'\rightarrow E,\Omega|\vec{r}')}_{\text{collision kernel}}\,dE'\,d^{2}\Omega'+\underbrace{Q(\vec{r}',E,\vec{\Omega})}_{\text{source term}}\right]\times\cdot\underbrace{T(\vec{r}'\rightarrow\vec{r}|E,\Omega)}_{\text{transition kernel}}\,d^{3}r'$$

where the different contributions can easily be singled out: the contribution from particles generated at point r' with initial energy E' and direction Ω' which final energy and direction after collision are respectively E and Ω (the particle energy and direction being modified by the collision kernel C) and propagated from point r' to point r by the transition kernel T. Additionally, the source term $Q(r', E, \Omega)$ corresponds to particles generated at r' with energy E and direction Ω that are propagated from point r' to point r by the transition kernel. This source term can be defined as

$$Q(\vec{r},E,\vec{\Omega})=\begin{cases}S(\vec{r},E,\vec{\Omega}) & \Leftrightarrow\text{Fixed Source}\\ S(\vec{r},E,\vec{\Omega})+\int\Psi(\vec{r},E',\vec{\Omega}')\underbrace{F(E',\vec{\Omega}'\rightarrow E,\vec{\Omega}|r)}_{\text{fission ``operator''}}dE'd^{2}\Omega' & \Leftrightarrow\text{Fixed Source + Fission}\\ \frac{1}{k}\int\Psi(\vec{r},E',\vec{\Omega}')F(E',\vec{\Omega}'\rightarrow E,\vec{\Omega}|r)dE'd^{2}\Omega' & \Leftrightarrow\text{Eigenvalue}\end{cases}$$

Defining for the sake of abbreviation of the notation

$$P\equiv(\vec{r},E,\vec{\Omega})$$

$$dP\equiv d^{3}r\,dE\,d^{2}\Omega$$

Then, the transport kernel $K(P', P)$ can be defined as

$$K(P',P)\equiv K(\vec{r}',E',\Omega'\rightarrow\vec{r},E,\Omega)=C(E',\Omega'\rightarrow E,\Omega|\vec{r}')\cdot T(\vec{r}'\rightarrow\vec{r}|E,\Omega)$$

Furthermore, being Ψ_i the density of particles entering the ith collision at point P, as pointed out in Lux and Koblinger (1991), the collision density at point P can be expanded in a Von Neumann series as

$$\Psi(P)=\sum_{i=0}^{\infty}\Psi_i(P)$$

with

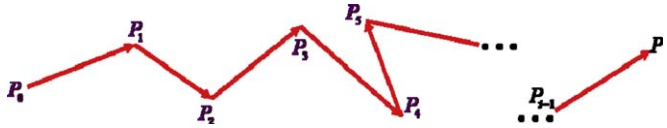
$$\Psi_0(P) = \int Q(P') \underbrace{T(P',P)}_{\text{transition kernel}} dP'$$

Then, it can easily be obtained that the following equation holds

$$\Psi_i(P) = \int \Psi_{i-1}(P') \underbrace{K(P',P)}_{\text{transport kernel}} dP'$$

being $\Psi_{i-1}(P')$ the probability density for the occurrence of the $(i-1)$th collision at P' and $K(P', P)$ the probability that a $(i-1)$th collision at P' will result in the ith collision taking place at P.

A history is then a sequence of states $(P_0, P_1, P_2, \ldots, P_{i-1}, P_i)$



and the transport equation stated in terms of the neutron collision density can then be recursively written as

$$\Psi_i(P) = \int\int\int \ldots \int \Psi_0(P_0) K(P_0 \to P_1) \times K(P_1 \to P_2) \ldots K(P_{i-1} \to P)\, dP_0\, dP_1\, dP_2 \ldots dP_{i-1}$$

This equation contains the essence of the Monte Carlo approach to perform radiation transport:

- Generate a sequence of states, $(P_0, P_1, P_2, P_3, \ldots)$ [i.e., a history].
- Randomly sample from the probability distribution function for the source in order to obtain $\Psi_0(P_0)$.
- Randomly sample from probability distribution function $K(P_{k-1} \to P_k)$, $k = 1, \ldots i$ in order to perform the ith transition.
- Generate estimates of results, R, by averaging over N histories and recalling the essence of Monte Carlo integration,

$$R = \int R(P)\Psi(P)\, dP \approx \frac{1}{N}\sum_{n=1}^{N}\left(\sum_{i=1}^{\infty} R(P_{i,n})\right)$$

Besides Lux and Koblinger (1991), an excellent and exhaustive overview of the Monte Carlo methods applied to solve the neutron Boltzmann transport equation can be found in Brown (2005).

4.2.2. Important issues on Monte Carlo simulation methods

Computer programs performing Monte Carlo simulations have to deal with the following issues:

- *Probability distribution functions* (pdf): the physical system must be described by a set of probability density functions.
- *Random number generators*: methods for generating random numbers uniformly distributed on the interval [0, 1] must be available and implemented.
- *Sampling rules*: a (set of) prescription(s) for sampling from the specified pdf's must be provided and implemented, namely:
  - from *analytic* pdf's (normal, exponential, Mawellian, etc.)
  - from *tabulated* pdf's (angular and energy spectra, among others)
- *Scoring* (*or tallying*): the outcomes must be accumulated into overall tallies or scores for the quantities of interest.
- *Error estimation*: assessment of the statistical error (variance) as a function of the number of trials and other quantities.
- *Variance reduction techniques*-methods for reducing the variance in the estimated solution in order to reduce the computational time required for the Monte Carlo simulations to provide meaningful physics results.
- *Parallelization and vectorization*: algorithms and methods that allow Monte Carlo methods to be implemented efficiently on advanced computer architectures must be developed and implemented.

4.3. Monte Carlo versus deterministic

The following table displays succinctly the main advantages and disadvantages of using the Monte Carlo and the deterministic methods to perform the simulations of a physical system.

Method	Advantage	Disadvantage
Monte Carlo	Detailed representation of geometry	Long computation time
	Accurate energy treatment	"Limited" information
	"Small" memory	Difficulty in using variance reduction
Deterministic (S_N)	Fast	Spatial discretization
		Angular quadrature order
	Detailed information	Approximate representation of geometry
		Approximate representation of energy treatment
		Large memory requirements

4.4. Hybrid methods

Monte Carlo and discrete ordinates methods are based on completely different mathematical (and philosophical) approaches. Yet, both methods solve the same physical problem.

The communities of experts performing Monte Carlo and deterministic calculations exist since several decades. In the past, they were nearly disjoint, and have had no influence on one another. Advances in Monte Carlo methods had no effect on deterministic methods—and vice versa—until recently.

However, in the last 10–15 years, researchers have learned that it can be advantageous to use a deterministic code to calculate the biasing parameters for a complicated Monte Carlo simulation. Therefore, a third category of methods has emerged in recent years, consisting of the merging of Monte Carlo and deterministic techniques, to obtain new *hybrid* computational methods that enhance the strengths and suppress the individual weaknesses of the individual Monte Carlo and deterministic (S_N) approaches. Nevertheless, in spite of its great potential, this category of hybrid methods remains still largely unexplored.

5. Open and hot issues

5.1. High-energy transport

As previously alluded to, the simulation of high-energy (starting in the hundreds of MeV) proton- and neutron-induced nuclear reactions in thick targets became the issue for different applications. In these applications, hadron, photon and even electron-positron transport simulation is required in order to compute the build-up and development of cascades of interactions triggered by incoming protons or neutrons impinging on a material and the secondary particles (protons, neutrons, mesons, fragments, photons) produced during the so-called *spallation reactions*.

Considering the scarcity of available experimental and evaluated data for some materials in these energy ranges, theoretical physics models must be used in order to model the nuclear reactions and to provide the predictions for the differential

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

cross-sections that are used to compute the neutral and charged-particle production in the final state.

The degree of reliance of these models on different parameters specific to the model itself varies from one model to another. These parameters are often used to "tune" and adjust the model predictions to available experimental data or even to the predictions of other models.

As described in Kadi et al. (2001) the generally accepted scheme for describing the hadron (proton and neutron) induced spallation reactions and associated nuclear interactions at high energies assumes the development of an *intranuclear cascade* (nucleon–nucleon interactions inside the nucleus) followed by intermediate *pre-compound stages* including fragmentation, break-up and equilibrium steps, treated by different models. Neutron evaporation (release of neutrons) and high-energy fission are among the steps by which the formed *compound nucleus* can proceed during de-excitation. The different particles and fragments (protons, neutrons, mesons, deuterium, alpha, tritium, etc.) produced and released from the nucleus during the intranuclear cascade then develop an *internuclear cascade* and also induced other inelastic reactions that further contribute to the production of multiple final state particles.

As for the specific applications which use a proton beam impinging on a thick target in order to produce the high neutron fluxes, it is well established (with supporting experimental data) that

- spallation neutron multiplicity varies with the material and, for a given material, linearly with the energy of the incoming proton in the range from a few hundreds of MeV up to a few GeV,
- the neutron yield normalized to the proton energy exhibiting saturation effect after a few GeV,
- the energy spectrum of the spallation neutrons is harder than typical fission spectra, with an average energy ranging from 3 to 4 MeV for the majority of materials of interest.

For the coming years, the improvement of the accuracy of high-energy hadronic transport will require new high-quality experimental data, the systematic validation and benchmarking of existing theoretical models and new evaluations of data sets for the energy ranges, types of particles, interactions and materials considered in the different innovative and emerging applications previously described.

5.2. On Monte Carlo simulations

The big issue to be solved concerns the time needed to perform computations in complex systems, for both the type of the physics and the geometry. Speed-up is therefore the issue! This can be achieved by sophisticated variance reduction techniques and capabilities, already present in the majority of the state-of-the-art Monte Carlo codes but their manipulation often leads to results that the majority of the users cannot fully implement (e.g., choice of importance) understand (e.g., particle weighs) and interpret (e.g., tallies results are often of difficult analysis). Automated variance reduction techniques could be one feature to be offered by Monte Carlo programs, although the underlying "black box" user-utilization could seem contradictory to the ultimate objective to be attained. Parallel computing is certainly another key aspect that will allow to speed-up Monte Carlo calculations; however, a major effort should be devoted by developers in order to improve the user-friendliness of its utilization, besides major developments both at the hardware and software level.

Another big issue, particularly relevant for the innovative and future nuclear technology systems (power reactors, ADS, etc.) is the time dependence (and full 3-dimensional) inherent to the transient thermal-hydraulic behavior of the system, to fuel burn-up and kinetics calculations. These are particularly important for the safety assessment and for the improved understanding of the safety sequences of these systems.

Other important topics and developments that could be driven by different applications, namely on Medical Physics and medical applications of radiations would be the development of capabilities that would allow to easily import into Monte Carlo programs imagiological data from organs. This is partly achieved in some of the existing programs.

CAD driven input preparation could also be requested by different applications.

New tallying features and capabilities are also items of potential future requests.

5.3. On deterministic calculations

Two of the major issues to be solved are related to the geometrical description (granularity and coarseness of the spatial and angular discretizations) and the physics (energy groups considered). However, improvements in both topics reach one of the major limitations in the hardware (the memory of computers).

In order to overcome and avoid the shortcomings of deterministic *vis-a-vis* Monte Carlo calculations the following requirements are mandatory:

- as granular as possible a description of the geometry, that implies
  - angular discretization ⇒ higher N (S_N)
  - very fine meshes and spatial discretization
- as granular as possible a description of the "physics", that implies
  - energy discretization (higher G)
- efficient and accurate cross-section preparation utility programs
- "Efficient", accurate and "stable" differencing schemes (speed-up of the convergence of the solutions)
- time-dependent and efficient 3-dimensional computations

Assuming that hardware limitations would be solved, the ultimate limitation will always reside in the physics, considering the high-energy processes involving both charged and neutral particles and the associated hadronic and electromagnetic interactions associated.

6. Conclusions

To solve 3-dimensional, real-world particle transport problems *accurately* and *efficiently*, hybrid methodologies and parallel algorithms are needed. Additionally, as noticed in Cullen (2002) over the years there was an imbalance between the efforts devoted to code development and those aiming at assessing the quality of the data used by Monte Carlo and deterministic radiation transport codes and solving the problem of the scarcity of the experimental and/or evaluated data available. The latter would call for the undertaking of new experimental campaigns, for the benchmarking of the existing physics models and for the intercomparison of theoretical models; all of these efforts imply a considerable amount of financial and human resources.

Computation of the time-dependency of the systems is a major issue for the coming years in order to allow accurate simulation of

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022

the transient behavior in nuclear systems and to perform, among others, detailed thermal-hydraulic and burn-up calculations in nuclear systems. The assessment of the time evolution of the activation products in accelerator and target systems is another example pointing to the need to perform effective time-dependent Monte Carlo and deterministic computations.

As pointed out in OECD (2005), with a declining number of nuclear data evaluators in the world and an increasing demand for high-quality data, there is a risk that evaluators will concentrate on producing new nuclear data to the detriment of developing new models and methods for evaluating existing data. There is a need to explore innovative approaches and new techniques to nuclear data evaluation in order to meet the requirements of the emerging nuclear applications.

Acknowledgements

Special thanks to Enrico Sartori and to José Salgado for their useful comments and helpful suggestions that certainly contributed to improve the clarity of the text and its contents.

References

Brown, F., 2005. "Monte Carlo Advances & Challenges," first lecture at the 2005 Frederic Jolliot/Otto Hahn Summer School, Karlsruhe, Germany.

Chadwick, M., et al., 1997. Nuclear data for nuetron therapy and radiation protection. In: Proceedings of the Eighth Symposyum in Neutron Dosimetry, Radiation Protection Dosimetry, Vol. 70, pp. 1–12.

Cullen, D.E., 2002. TART: Monte Carlo Radiation Transport in Industrial Applications, Report UCRL-JC-134196.

Felcini, M., et al., in press. Radiation and safety issues in the design of the EURISOL multi-megawatt target. In OECD Proceedings of the Eighth Specialists Meeting on Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF-8), Pohang, Korea, 22–24 May 2006, OECD Publication.

Giraud, B., et al., 2005a. PDS-XADS: General Synthesis Report of XADS Preliminary Design Studies and Needed R&D, Document DEL/05/086, Technical and scientific report of the EU-funded project PDS-XADS.

Giraud, B., et al., 2005b. Technical Option Report on the Gas-Cooled XADS, document DEL/04/062, Technical and scientific report of the EU-funded project PDS-XADS.

Haghighat, A., 2004. Advances in Particle Transport Methods and Future Needs and Directions, Invited talk at the Tenth International Conference in Radiation Shielding (ICRS-10), Madeira Island (Portugal).

Hirayama, H., in press. Inter-comparison of medium-energy neutron attenuation in iron and concrete. In: OECD Proceedings of the Eighth Specialists Meeting on Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF-8), Pohang, Korea, 22–24 May 2006, OECD Publication.

James, F., 1968. "Monte Carlo Phase Space," CERN report 68-15.

James, F., 1980. "Monte Carlo Theory and Practice," CERN Data Handling Division report DD/80/6.

Kadi, Y., et al., 2001. Simulation of accelerator driven systems. In: Proceedings of the "Workshop on Hybrid Nuclear Systems for Energy Production, Utilisation oF Actinides and Transmutation of Long-Lived Waste," Trieste.

Lewis, E., Miller Jr., E., 1993. Computational methods of neutron transport, American Nuclear Society.

Lux, I., Koblinger, L., 1991. Monte Carlo Particle Transport Methods: Neutron and Photon Calculations. CRC Press, Boca Raton, FL.

Maschnik, S., et al., 2000. Models and codes for intermediate energy nuclear reactions (an overview). Models and codes for spallation neutron source". In: Proceedings of the Fifth Meeting on Simulating Accelerators Radiation Environment (SARE-5), Paris, France, 17–18 July 2000.

O'Dell, R.D., Alcouffe, R.E., 1987. Transport Calculations for Nuclear Analysis: Theory and Guidelines for Effective Use of Transport Codes," report LA-10983-MS.

OECD Proceedings of the Workshop on "Perspectives on Nuclear Data for the Next Decade," Bruyères-le-Chatel, France, 26–28 September 2005.

Orsi, R., Private communication.

Pelliccioni, M., 2000. Overview of fluence-to-effective dose and fluence-to-ambient dose equivalent conversion coefficients for high energy radiation calculated using the FLUKA code. Radiation Protection Dosimetry 88, 279.

2005 Recommendation of the International Commission on Radiological Protection—Summary of Recommendations, Relatório preliminar do ICRP, 2005.

Reitz, G., 1993. Radiation environment in the stratosphere. Radiation Protection Dosimetry 48–1, 5–20.

Rubbia, C., et al., 1993. An Energy Amplifier for Cleaner and Inexhaustible Nuclear Energy Production Driven by a Particle Beam Accelerator. CERN preprint CERN-AT-93-47.

Rubbia, C., et al., 1995. Conceptual Design of a Fast Neutron Operated High Power Energy Amplifier. CERN preprint CERN-AT-95-44.

Rubbia, C., et al., 2001. A European Roadmap for Developing ADS for Nuclear Waste Incineration.

Sakamoto, Y., et al., in press. Standard data of dose conversion coefficients in Japan. In: OECD Proceedings of the Eighth Specialists Meeting on Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF-8), Pohang, Korea, 22–24 May 2006, OECD Publication.

Salvatores, M., 2002. "The Physics of Subcritical Multiplying Systems," in: "Nuclear Science in Europe: Impact, Applications, Interactions," NuPECC Report.

Schraube, H., 2003. How large is the exposure of pilots, aircrew and other frequent flyers to cosmic radiation, GSF (Institute of Radiation Protection) report.

Spallation Neutron Source—Preliminary Safety Assessment Document, 2000.

Thomas, R.H., 2004. Standards for Standard Makers? A Testing time" (invited paper). Radiation Protection Dosimetry 109–4, 277–289.

Vanneri, F., et al., 1993. Accelerators address nuclear waste problems. In: Physics World, pp. 40–45, (August 1993).

Vervier, J., et al., 2003. The EURISOL report—a Feasibility Study for a European Isotope Separation On-Line Radioactive Ion Beam Facility, report to the European Commission, published by GANIL.

Please cite this article as: Vaz, P., Neutron transport simulation (selected topics). Radiat. Phys. Chem. (2009), doi:10.1016/j.radphyschem.2009.04.022