Radiation Physics and Chemistry 130 (2017) 186–195

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

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

Monte Carlo simulation of random, porous (foam) structures for neutron detection

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HIGHLIGHTS

- Description and testing of novel Dynamic Path Generation Monte Carlo technique.
- Characterization of the physical structure of RVC foams with various porosities.
- Preliminary validation of Dynamic Path Generation by comparison to MCNP6.
- Optimization study of simulated B_4C-coated RVC foam materials.

ARTICLE INFO

Article history:
Received 5 January 2016
Received in revised form
22 August 2016
Accepted 27 August 2016

Keywords:
Monte Carlo
Neutron detection
RVC foam
Boron-carbide
Lithium-fluoride

ABSTRACT

Porous media incorporating highly neutron-sensitive materials are of interest for use in the development of neutron detectors. Previous studies have shown experimentally the feasibility of ^{6}LiF-saturated, multi-layered detectors; however, the random geometry of porous materials has limited the effectiveness of simulation efforts. The results of scatterless neutron transport and subsequent charged reaction product ion energy deposition are reported here using a novel Monte Carlo method and compared to results obtained by MCNP6. This new Dynamic Path Generation (DPG) Monte Carlo method was developed in order to overcome the complexities of modeling a random porous geometry in MCNP6. The DPG method is then applied to determine the optimal coating thickness for $^{10}B_4C$-coated reticulated vitreous-carbon (RVC) foams. The optimal coating thickness for 4.1275 cm-thick $^{10}B_4C$-coated reticulated vitreous carbon foams with porosities of 5, 10, 20, 30, 45, and 80 pores per inch (PPI) were determined for ionizing gas pressures of 1.0 and 2.8 atm. A simulated, maximum, intrinsic thermal-neutron detection efficiency of $62.8 \pm 0.25\%$ was predicted for an 80 PPI RVC foam with a 0.2 μm thick coating of $^{10}B_4C$, for a lower level discriminator setting of 75 keV and an argon pressure of 2.8 atm.

1. Research motivation

Porous materials are currently under investigation for use as thermal-neutron detectors. Highly neutron-absorbing materials that react with thermal neutrons and produce energetic ions as reaction products must be incorporated in the porous material to enable the detection of neutrons. The charged-particle reaction products ionize gas within the pores of and surrounding the porous material. This ionization is then collected at the detector electrodes to produce an electronic pulse that records the neutron interaction event (Tsoulfanidis, 1995). Typically, ^{10}B or ^{6}Li are incorporated into the porous material either by impregnation or as a coating (Nelson et al., 2012).

Porous materials consist of struts and pores. Struts provide the structural support for the porous material and are composed of solid material which connect to form the support network. Pores consist of the void between struts in a porous material, and in the case of open-cell materials, are filled by any fluid within which the porous material is immersed. A generic example of a porous material is shown in Fig. 1. The original bubbles that exist during the manufacture of the porous material form a perfectly-packed, three-dimensional array of similarly sized bubbles (ERG Aerospace Corporation, 2011). After solidification of the porous material, struts are formed between pores as the result of the intersection of adjacent bubbles. The porous materials of interest in the present work are isotropic in nature, such that neutrons, on the average, encounter the same total thickness of the strut material, per unit path length of travel, regardless of the directions the neutrons travel through the material.

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http://dx.doi.org/10.1016/j.radphyschem.2016.08.021
0969-806X/

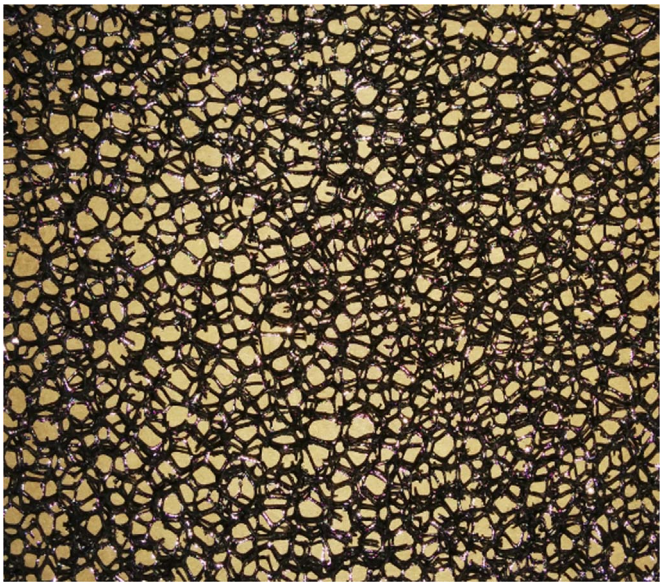

Fig. 1. Porous materials are composed of an interconnected network of solid struts which surround the gas-filled pores (ERG Aerospace Corporation, 2011).

Numerous porous materials are presently under investigation for possible use as neutron detectors; however, open-cell foam-based materials are of particular interest because of their extremely low cost and ease of fabrication (Nelson et al., 2012). Previous studies have investigated aerogels, ^{6}LiF-impregnated polyethylene foams, (Nelson et al., 2011) and boron-coated, reticulated vitreous-carbon (RVC) foams experimentally (Lavelle et al., 2013). Experimental work could be guided by the simulations capable of comparing various types of foam and geometric foam parameters. Although some attempts have been made to simulate such porous materials (Nelson et al., 2011), these earlier studies have suffered from one of two potentially limiting assumptions. First, ionization of the gas within the pores, inside the bulk of the material was neglected despite such ionization being critical to the intrinsic neutron detection efficiency (Lavelle et al., 2013). Second, although porous materials are composed of a heterogeneous system of pores and struts, past work approximated the porous materials by mass-conserving homogenization (Nelson et al., 2012). The results of this previous work have done well to advance the experimental progress towards a porous neutron detector; however, a more accurate simulation method is necessary.

In order to account for the ionization within the internal pores, particle transport must be modeled using an explicit representation of the complicated foam geometry. However, the random nature of heterogeneities comprising the interior of porous materials greatly complicates the development of a fully-defined geometric model for use in commonly used particle transport software packages. Specialized methods to simulate Monte Carlo ion transport can overcome some of the limitations of particle transport software packages. Two different methods were used in the present work to simulate porous materials for use as neutron detectors. First, a script was written in Python to generate an input file for use in the Monte Carlo Neutral Particle version 6 (MCNP6) software package. MCNP6 is a general-purpose Monte Carlo simulation code used for neutral particle, electron, and ion transport (Tsoulfanidis, 1995). A simple benchmark porous material problem was solved using MCNP6 and a novel Dynamic Path Generation (DPG) Monte Carlo method, developed and described here. The DPG method can accommodate more complex problems involving random heterogeneities. In lieu of adequate experimental data, a benchmark problem was solved with both methods to validate the DPG method.

2. Monte Carlo simulation methods

While previous studies have made progress in the simulation of porous media for neutron detection, most methods have required unrealistic assumptions about the material and, typically, neglect ionization occurring within the pores inside the bulk of the porous material (Lavelle et al., 2013). The amount of ionization which occurs within the pores inside the bulk of a porous material is one of the possible advantages of these materials but depends greatly on the geometry within the foam material, specifically the strut and pore dimensions. Simulations that can closely predict the response of a neutron reactive porous material to a thermal-neutron flux were developed here using MCNP6 simulations to serve as benchmarks for a new DPG method for treating random media.

Monte Carlo simulation is commonly used to solve complex particle transport problems (Dunn and Shultis, 2012). In the present case, the problem involves complex geometries and involves coupled neutron and ion transport calculations. The MCNP6 software package was the first choice when considering the simulation of porous materials for neutron detection. Both MCNP6 and custom Monte Carlo simulations have been used to predict the effectiveness of coated diode neutron detectors in the past (Shultis and McGregor, 2009). Although porous materials are composed of a heterogeneous system of pores and struts, past work has approximated porous materials by homogenization (Nelson et al., 2011; Lavelle et al., 2013). Homogenized simulation can adequately approximate the total neutron absorption in a porous medium, but cannot accurately estimate the ionization in the fill gas, which is the primary consideration of this work.

2.1. Dynamic path generation Monte Carlo simulation

One difficulty in simulating porous materials is the random nature of the interior heterogeneities. The isotropic distribution of pores of various sizes within the porous material makes the creation of a three-dimensional geometric model difficult and must first be characterized.

2.1.1. Geometric approximations and sampling distributions

The two types of foams that were simulated for the present work were characterized using a scanning electron microscope (SEM) to measure the strut thickness, pore diameter, and neutron-reactive coating thickness (where applicable) in numerous locations. After imaging LiF impregnated foam samples, the struts were approximated as right circular cylinders. In contrast, the RVC foam samples were observed to possess struts which were shaped approximately like equilateral triangular prisms. The thickness of the struts was measured from the center of each side of the strut as depicted in Fig. 2. The neutron-reactive coating thickness was also measured for struts as shown in Fig. 3. Both LiF impregnated foam and RVC foam had gas-filled pores that resembled circular openings, the diameter of which was measured from several locations, as illustrated in Fig. 4. The measurements to characterize the critical geometric parameters were repeated over numerous locations for foam samples with six different pore densities (5, 10, 20, 30, 45, and 80 pores per inch (PPI)). An average value and standard deviation were calculated from the SEM measurements, summarized in Table 1. A histogram of measured pore diameters for an 80 PPI foam sample is shown in Fig. 5. The values listed in Table 1 were based on a relatively small number of measurements (typically <50 measurements). The error associated with these measurements is noticeable and is captured in the standard