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MCNP5 code in radioactive particle tracking

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1. Introduction

ABSTRACT

Radioactive particle tracking techniques have been widely applied in the field of chemical engineering, especially in hydrodynamics in multiphase reactors. In classical approach, the phenomenological model is used to simulate the number of counts measured by the detector and then the tracer position is reconstructed by solving a minimisation problem between the measured events and the mentioned model. The paper presents an original algorithm for reconstruction of the tracer position during the radioactive particle tracking based on the Monte Carlo N-Particle code version 5. The validation of the proposed algorithm is evaluated for two cases: 'ideal' and physically realistic. The advantages of the new algorithm are demonstrated.

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The radioactive particle tracking (RPT) technique is based on tracking of the motion of a single radioactive particle in a volume of interest. The radioactive particle should have physical properties identical to the ones of the investigated flow. Nowadays, radioactive chemical elements such as Sc-46, Co-60 or other gamma-ray-emitting isotopes are widely used to track the motion in single or multiphase systems.

Instantaneous particle positions are identified by monitoring radiation intensities measured by detectors arranged in different positions around the volume (vessel). In order to reconstruct the position of the particle, a calibration procedure is needed. The calibration allows to consider the intensities measured at the detector as a function of coordinates of the particle. It is not feasible to carry out the calibration procedure by direct experimental measurements because of a large number of points, which must be considered. Generally, this number depends on the number of detectors, the dimensions of the volume (vessel) and requirement accuracy, although even a simple RPT system requires more than several thousand points for the calibration procedure.

In the last decades, various reconstruction algorithms have been developed to estimate particle position inside a vessel in time. These algorithms include a weighted regression scheme (Devanathan et al., 1990), a modified weight regression scheme (Luo et al., 2003; Rados et al., 2005), cross correlation technique (Bhusarapu et al., 2005) and the Monte Carlo approach (Larachi et al., 1994; Blet et al., 2000; Roy et al., 2002; Doucet et al., 2008).

Comparing with other algorithms, the algorithms based on Monte Carlo approach (discrete photon models) result in better particle position estimation accuracy since they model real stochastic nature of photon transport. These algorithms are based on estimating the total efficiency of a scintillation detector for photons emitted from a radioactive point source.

The well-known algorithms applying Monte Carlo procedures are based on rigorous phenomenal model proposed by Beam et al. (1978). However, this model is a simplified model of radioactive transport. Thus, it mainly considers the photoelectric effect and excludes other types of interaction of photons with matter, such as scattering effects. Furthermore, it only considers photon transport in a volume limited to the solid angle determined by the detector when seen from the particle's perspective. Another important limitation of previous works stems from limited computing power of obsolete workstations now, incapable of performing large-number calculations.

The aim of this paper is to introduce the utilisation of the MCNP (Monte Carlo N-Particle transport) code version 5 (MCNP User Manual, Version 5, 2003) in the performance calibration procedure. Additionally, we present an original algorithm for mapping counts into the particle position coordinates.

The verification of the proposed calibration procedure was done for non-invasive flow mapping of the hydrodynamics in a bubble column employing fifteen NaI detectors. Through the example of this proposed implementation, we demonstrate how MCNP code can be used for performance calibration procedure for the experiment.

2. The MCNP5 model

In the last few decades, several works have been undertaken in order to improve RPT resolution and sensitivity, either by improving

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the design of the experiments or by selecting the appropriate isotope for the tracer. The well-known RPT methods reconstruct the tracer position through solving a minimisation problem between the measured counts and the *rigorous phenomenological model* proposed by Beam et al. (1978) and thereafter applied by Larachi et al. (1994). This model relates the position of the emitter to the number of counts recorded by each detector surrounding the system. The detectors measure different levels of radiation depending on the position of the emitter. Using an appropriate model, the exact location of the tracer can then be obtained.

The location of the tracer is represented in Cartesian coordinates by $\mathbf{p}(x,y,z) \in V$, and the function $C_i(\mathbf{p},t)$ expresses the number of counts measured by the *i*th detector at position \mathbf{p} of the tracer at time *t* in the following manner (Beam et al., 1978):

$$C_{i}(\mathbf{p},t) = \frac{T v R \phi \xi_{i}(\mathbf{p},t)}{1 + T \tau v R \phi \xi_{i}(\mathbf{p},t)}, \quad i = 1, \dots, n$$
(1)

where *T* is the dwell time, τ is the dead-time of the detectors, *R* is the source activity, *v* is the number of photons emitted by disintegration, ϕ is the photopeak-to-total ratio and $\xi_i(\mathbf{p}, t)$ is the efficiency of *i*th detector with respect to a given position \mathbf{p} , *n*—is the number of detectors.

To compute the efficiency of the *i*th detector with respect to a given position **p**, a numerical approach based on a Monte Carlo method is widely used (see Larachi et al., 1994; Roy et al., 2002; Doucet et al., 2008). The method consists of determining a corresponding solid angle Ω for each detector and generating many random photon histories.

Contrary to the well-known methods (Larachi et al., 1994; Roy et al., 2002; Doucet et al., 2008), which use the Monte Carlo method for generating random photon histories *in the direction of each detector*, the MCNP code gives excellent possibilities to obtain the number of counts measured by all detectors at tracer position **p**, $C_i(\mathbf{p},t)$, i=1,...,n, simultaneously without making it necessary to use Eq. (1). The MNCP5 code allows generating photon histories from a tracer particle throughout the entire volume, i.e. not limited to a solid angle only (see Fig. 1). This implies that it is not necessary to perform calculations for the *distance-count map* for each detector separately.

Furthermore dominant mechanisms of photon interaction with matter are included in the MCNP5 code, including: Rayleigh scattering, photo-electric absorption, X-ray fluorescence, Auger effect, Compton scattering, pair production, multiple scattering and ionisation. Most of these are dominant mechanisms for gamma-ray transport. Additionally the MCNP5 package delivers detailed information on the transport and energy deposition,



Fig. 1. MCNP5 code in a RPT technique: tracer particle releases photons throughout the volume (not only at solid angle of 4π).

including energy and angular distributions of emerging particles, depth–dose distribution, deposited energy distribution, etc.

The first step in using the MCNP5 code is to define the 3D geometry of the RPT tracking system, including the percentage and density of all materials.

The next step is to model the radioactive tracer source. Since the diameter of a tracer is roughly equal to several mm, point approximation can be chosen for modelling purposes.

The third step is simulation of the detector type. MCNP code automatically creates standard summary information that gives the user a better insight into the physics of the problem and the adequacy of the Monte Carlo simulation including: a complete accounting of the creation and loss of all tracks and their energy: the number of tracks entering and reentering a cell plus the track population in the cell; the number of collisions in a cell; the average weight, mean free path, and energy of tracks in a cell; the activity of each nuclide in a cell (that is, how particles interacted with each nuclide, not the radioactivity) and a complete weight balance for each cell. This standard summary information can be released using seven tally types (Shultis and Faw, 2006). The tallies are used to specify what type of information the user wants to gain from the Monte Carlo calculation. The MCNP5 code includes several types of tally cards to specify what type of information the user wants to gain from simulation.

In this work, we are interested in the counts recorded in each active volume of the detector. Tally type 8, allowing to record the energy distribution of pulses created in a detector, can be used to model each detector operation. Thus, type 8 tally records the energy of a scoring track in the energy bins. The energy bins correspond to the total energy deposited in a detector by each physical particle (history) that is analogous to a physical detector.

Since Monte Carlo results represent the average of contributions from many histories of primary photons to be generated during each simulation at a given photon energy, the choice of the number of primary photons *N* generated during each simulation plays an important role in Monte Carlo simulations. This number *N* should be adjusted so that all desired results would pass all ten statistical checks. These ten statistical checks are performed for each result with a *pass yes/no* criterion by the MCNP code (Shultis and Faw, 2006) and include estimated mean, relative error, variance of the variance and history score probability density function. The checks provide the user with more information about the statistical behaviour of the Monte Carlo calculations and can be used for estimation of their precision for a real RPT set-up in practice.

3. Reconstruction of the tracer position

The distance-count map generated during the calibration phase is next used to reconstruct the instantaneous position of the tracer particle as a function of time (i.e. particle Lagrangian trajectory). There are several particle position reconstruction algorithms implemented to reconstruct the best estimate of the particle position, such as a weighted least-squares algorithm, a wavelet-based position filtering, etc.

Because the calculations of the map of counts are *approximate* and they are done for selected tracer locations, a strategy must be devised to calculate the tracer position with minimum error.

To detect instantaneous position of the tracer particle, original reconstruction algorithm is proposed (see Fig. 2).

Before running the algorithm, the distance-count map $\{C_{i,j}^s\}, i = 1, ..., n, j = 1, ..., J_{max}$, where *n* is the number of detectors, and J_{max} is the number of simulated positions of the tracer, should be calculated for selected tracer locations $(x_j, y_j, z_j), j = 1, ..., J_{max}$ using corresponding MCNP5 codes.

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