MATHEMATICAL MODELING IN RADIATION PROCESSING

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This papers gives an overview of mathematical modeling in industrial radiation processing using electron beam, gamma and X-ray sources. Emphasis will be on Monte Carlo Transport Codes, which play an important role and are widely used.

The paper is organized in three parts: the first part deals with the basic requirements, features and examples of mathematical modeling tools and they are discussed in the context of their applicability for industrial radiation processing.

The second part of the paper presents several areas, where mathematical modeling has been successfully applied. The applications described include process design and verification, product qualification, throughput calculations and process capability analysis.

In the third part, important topics like benchmarking and verification of modeling results and the value of international interest groups is discussed. The paper concludes with recent developments like cluster hardware, enhanced graphics capabilities and GRID computing, which may boost the range of application in industrial irradiation processing even more in the future.

I. INTRODUCTION

Using mathematical models for calculating absorbed dose in industrial radiation processing is an emerging field showing encouraging results and increased acceptance in the radiation processing community.

Mathematical models may be divided into Monte Carlo, deterministic, semi-empirical and empirical models.[1] Monte Carlo methods, used as synonym for mathematical models in this paper, simulate the tracks of individual particles based on the detailed physics of the interaction of radiation in matter. In contrast to deterministic models which solve the partial differential equations of radiation transport, Monte Carlo sample the interactions as probability functions derived from cross section data or theoretical considerations. Energy losses of particles (mainly electrons and photons) in matter from different histories are summed to calculate the absorbed dose in a product volume.

Historically, a significant impact had the ground-breaking paper of Martin J. Berger, which laid the foundation of Monte Carlo methods for radiation transport[2]. Monte Carlo methods for radiation transport are predominantly used in areas where radiation dosimetry is difficult or impossible, like radiation therapy or space applications.

Today several Monte Carlo codes are available and used for industrial applications, like gamma (Co-60), electron beam or X-ray irradiation. The main field of application is the calculation of dose distribution in complex geometries for process design, product validation or process qualification.

Typical examples of available Monte Carlo codes are EGS, GEANT4, ITS or MCNPX which are distributed by national and international institutions. Refs. 2,3 give an excellent overview over existing computer codes and their availability .

II. OVERVIEW OF INDUSTRIAL APPLICATIONS

The use of ionizing radiation for industrial applications has a long (over 50 years) and successful track record. The biggest application of ionizing radiation is still the cross-linking of polymers with electron beam and the majority of the installed electron accelerators are used for irradiating wires, cables, tubes, tires or engineering plastics parts to improve their heat resistance and other functional parameters. This field of application is nowadays commonly referred as advanced material processing and it comprises also curing of inks or composites, grafting or semiconductor and gemstone treatment.

The second major strand of applications is associated with the capability of ionizing radiation to kill harmful microorganisms. In 1956 Ethicon, a Johnson & Johnson company, introduced industrial radiation sterilization and started an emerging field were ionizing radiation from gamma, electron beam or X-rays is used to sterilize medical devices, pharmaceutical products, decontaminate food packaging or sanitize food stuff.

An emerging field is also the use of ionizing radiation for environmental applications. Good examples are the cleaning of stack gas or destruction of environmentally harmful chemical compounds.

III. MOTIVATION FOR USING MATHEMATICAL MODELLING

The motivations for using mathematical modeling in industrial radiation processing are manifold. They include: facilitate process design, assessment of the uncertainty associated with a process, assistance and complementation of dosimetry and failure analysis.

Mathematical modeling can help to transform ideas to a process or a product. The computation of dose distribution by simulation gives insight into the process and allows to determine the optimal irradiation equipment and predicts process boundaries. As an example, lets consider the sterilization of medical devices with electron beam. The product must receive a certain dose D_{min} to guarantee sterility and shall not receive a dose above D_{max}, because otherwise the product may fail because of e.g. polymer degradation. Simulating the irradiation with a Monte Carlo code allows to predict the process window [D_{min}, D_{max}] and the dose at a reference position D_{ref}, which is needed to release the product in the routine process. Process parameters like beam energy and scanning configurations can be tuned, long before the irradiator is build. In addition it is possible to predict process throughput and hence evaluate the economics of the process.

Mathematical modeling on the other hand allows to assess the uncertainty of a process. The influence in the variation of beam energy or spectrum, product density or packaging configuration can be studied by running simulations with different parameter sets. This allows to assess type B uncertainty and therefore increases process stability and safety.

Mathematical modeling cannot and will not substitute dosimetry but it is a valuable tool to complement dosimetry. An example is the use of very low energy electrons ($E < 100$ keV). For this energy range and the associated extremely low penetration, the dosimeter is changing the radiation field and masking the true dose distributions. Combined information from modeling together with the dosimeter response allows to address dosimeter calibration issues at very low energies.[4]

Finally, if deviation from process specifications occur, mathematical modeling is often capable to track down the reason for the nonconformity and initiate corrective actions.

IV. REQUIREMENTS FOR MONTE CARLO TOOLS

All Monte Carlo codes show the following basic building blocks:

a) Geometry and material input
b) The physics engine which does tracking and scoring
c) The output module, which presents the results in a numerical or graphical way.

The requirements for Monte Carlo codes for industrial processing will be categorized according to these building blocks.

The irradiation and product geometry input and the specification of the associated materials is a major task when implementing a Monte Carlo applications. Historically the geometry and material input was done via text files. This method is ideal for small application comprising only few materials and simple geometry. For advanced simulations using real product with complex geometries, the textual method is getting difficult, time consuming and error prone. Some codes like GEANT4 (Ref.5) use a programmatic way to define geometry and materials. This method is very powerful, because the geometry is not specified but described in a high level computer language and as a results, very compact code may define a complex irradiator and product. On the other hand, this methods needs programming skills and advanced training. Both methods demand validation of the geometry input, which can be performed by inspecting the graphical output or by using specialized tools, which check e.g. for overlapping geometries and other faults. The optimal way for data input, is the direct use of 3D-CAD files from product design. This method however needs defined interfaces and the incorporation of material information in the files. While several promising attempts are already made, direct geometry input is still under development and we may see exciting possibilities in the near future. A possible bottleneck we are running into is the overwhelming complexity of industrial type geometries. Simulating any small detail of a design, may blow the capability of the simulation concerning memory usage and model execution time. Therefore expert knowledge, which details in the product geometry affect the dose distribution considerable and must be part of the model, will still be necessary.

Summarizing, a mathematical model shall have the possibility of a fast, cost efficient geometry and material input and a mean to validate the geometry before use.

The physics engine which is the central part of the Monte Carlo tools must be parameterized by the user before executing the model. These parameters include the step size of particle tracking or energy and range thresholds for particles to be tracked. Some tools also allow to switch on/off different interaction types, so special care must be taken and expertise and training is mandatory before use. To summarize, a tools should have a transparent way to parameterize the physics engine and training should be available. In addition the model shall be validated for its intended use (energy regime, accuracy requirement) and the validation sufficiently documented.

Because the uncertainty of the Monte Carlo model is decreasing with 1/√N, where N is the number of simulated events (called histories), a sufficient number of events must be run to get meaningful results. Typically more than 10 million events are necessary for medium type problems. Despite the use of ever more powerful processors, this may take a considerable amount of time, with execution times of hundreds of hours on a single personal computer. So execution time on the target hardware available has to be evaluated, because it may constitute a severe constraint on the industrial applicability of mathematical modeling. The opportunity to using clusters and the GRID is briefly described in section 7 of this paper.
To reduce the number of events required for a particular problem "variance reduction techniques" were developed ever since the Monte Carlo method is used. Variance reduction means in this context, that methods are applied, which decrease execution time without reducing accuracy. This may be done e.g. by importance sampling, where particle tracks towards a certain directions or regions are statistically enhanced. Monte Carlo models used in industrial applications should have the possibility to implement variance reduction methods, however their use needs a lot of experience and experimental validation.
Post-processing and output of the results is the last step of running a mathematical model. This may be easy for simple numerical output, but industry usually demands high quality 3D- graphics. These high expectations call for sophisticated tools, which demand considerable training to use and powerful interfaces to make data transfer safe and efficient.

V. EXAMPLES

Examples of using mathematical models, especially Monte Carlo methods are numerous and increasing. One dimensional problems, where the dose in beam directions is studied (depth dose curves) are simple to implement, yet very powerful and heavily used. As an example all depth dose curves found in ISO/ASTM 51649 (Ref. 6) were generated using the 1-dimensional Monte Code ITS 3.0.

An open program framework like GEANT 4 allows to address specialized problems, which are difficult to attack in other packages. For a process development study, the spectrum of 500 keV (monoenergetic) electrons after traveling a certain distance in air was of interest and the energy dispersion depending on the air gap they travel could be studied.

Other examples for the use of Monte Carlo codes are the irradiation of small structures, where dosimetry is not possible and the irradiation of partial shielded objects (Fig. 1). In this setup the shadowing effect of a thin (100 μm) steel slab is simulated in order to demonstrate the performance of the GEANT4 Monte Carlo code.

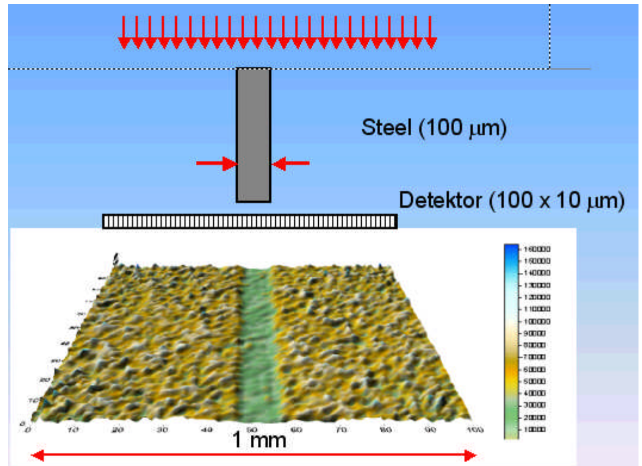

Fig.1 Dose distribution in a partial shielded object

VI. GUIDANCE

Modeling and simulation tools like Monte Carlo codes for radiation processing are powerful instruments to predict absorbed doses in order to assist and extend radiation dosimetry. Nevertheless these tools need extensive know-how to set up and interpret the output correctly. A good guidance document is ISO/ASTM 2232 where a road map for using mathematical tools is laid out. With the Radiation Process Simulation and Modeling User Group RPSMUG a professional collaboration to facilitate the use of mathematical modelling in industrial irradiation has been formed.[7] The major current focus of RPSMUG is the benchmark of several mathematical models against experiments in industrial electron beam and Co-60 irradiators.

VII. BOOSTING PERFORMANCE – CLUSTERS AND THE GRID

In the industrial world, were execution speed of Monte Carlo models may be a severe constraint, the use of distributed programming with PC clusters may become more common. Codes like MCNPX are known to run very well in a distributed LINUX environment and without the processing power of cluster hardware most of recent research on X-ray processing for industrial applications would not be possible.[8] In the future, pioneered e.g. in the L3 high energy physics experiment at CERN, the GRID concepts may become accessible for industrial users.[9]
While the Web is a service for sharing information over the Internet, the GRID is a service for sharing computer

power and data storage capacity over the Internet. Therefore it may be possible in the near future that industrial users design their model, execute it on the GRID and get the results in a few minutes. Naturally, before this ambitious and exiting scenario becomes true a bunch of problems like access policy, resource sharing, security, interfaces and standards have to be solved.

VIII. CONCLUSIONS AND OUTLOOK

Monte Carlo methods provide important tools for process development and control and have proven their benefit for problems in industrial irradiation applications. For one-dimensional problems like depth-dose distributions the TIGER code of the ITS package is an relatively easy to use tool. For complex geometries 3-dimensional models are available which match the demand of more ambitious industrial applications. However certain requirements are in place and RPSMUG, a newly formed users group represents a promising platform to coordinate activities in the emerging field of simulation and modeling for radiation processing.

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