Proceedings of the 2004 Winter Simulation Conference
R .G. Ingalls, M. D. Rossetti, J. S. Smith, and B. A. Peters, eds.

DYNAMIC RADIATION DOSE VISUALIZATION IN DISCRETE-EVENT NUCLEAR FACILITY SIMULATION MODELS

George H. Tompkins
Drew E. Kornreich
Robert Y. Parker
Andrew C. Koehler
Johnell M. Gonzales-Lujan
Robert J. Burnside

Los Alamos National Laboratory
P.O. Box 1663, MS F609
Los Alamos, NM 87545, U.S.A.

ABSTRACT

To improve its process modeling capabilities, Los Alamos has worked toward integrating dose modeling tools with advanced discrete-event simulation tools. To date, dose information for a model was preprocessed and then incorporated into a process model. In this paper, we describe a quantum improvement in our capabilities by linking a dose calculation kernel to the discrete-event modeling environment through the customizable routine capabilities provided by the Flexsim™ code. The Flexsim™ model uses ray-tracing routines to calculate the source and detector locations and determines the materials, thickness, and order of any shields between the source and detector. With this information, the dose calculation kernel is then able to calculate, in a post-processing setting, the associated dose. Thus, we are able to determine the time-varying and integrated exposure of workers to ionizing radiation, which will be integral to planning for future nuclear facilities in the DOE complex.

1 INTRODUCTION

Los Alamos, in its efforts to support its national security and energy-related missions, maintains facilities where nuclear materials, e.g., plutonium, are processed. Proper modeling of nuclear-materials facility operations must include the many constraints that are placed on these operations. Such constraints include the vast assortment of regulations imposed to ensure worker and public safety as well as security concerns. Some of the primary regulatory constraints are those related to the exposure to ionizing radiation that workers receive during the course of their work. The two key elements in estimating exposure are source strength and time. A discrete-event model is an ideal tool to provide statistically meaningful estimates of time.

1.1 Background – Radiation and Sources

Several key materials of national security and energy infrastructure interest are radioactive, that is, they spontaneously emit ionizing radiation of various forms. The rate of emission is statistically embodied in the half-life, defined as the time after which half of the radioactive atoms have decayed.

The primary particles emitted by radioactive atoms are alpha particles (a helium nucleus), beta particles (an electron), a gamma ray (energetic electromagnetic radiation), and neutrons. Alpha and beta particles are easily shielded; however, when radioactive atoms enter the body and then decay by alpha or beta emission, e.g., in the lungs, they are very hazardous. To address this issue, most handling operations occur in gloveboxes to contain the materials and prevent them from entering the body.

Because gamma rays and neutrons carry no electric charge, they are much more difficult to shield. Gamma rays are most often shielded with dense, high atomic number materials such as lead (often incorporated into a glovebox design). Neutrons are best shielded with materials containing hydrogen, as the hydrogen allows the neutrons to lose energy upon collision with the hydrogen, which makes them less harmful and also improves the chances that a neutron will be absorbed by a shield material.

The sources handled at Los Alamos generally consist of some form of plutonium, either as a metal, oxide, salt, or dissolved in a liquid. Plutonium decays by alpha particle emission and by spontaneous fission. If there are low atomic number materials chemically joined to the plutonium, e.g., oxygen or chlorine, the alpha particles can react with these atoms to produce neutrons in an alpha-n reaction. Spontaneous fission also produces energetic neutrons, and both decay forms produce gamma rays.

1.2 Previous Dose Estimating Work

In the past, Los Alamos has included dose estimates as one of the parameters to be studied in performing modeling of nuclear materials operations. However, such modeling has been relatively simplistic. In general, a dose calculation tool, such as an in-house code Pandemonium (Kornreich and Dooley 1999), is used to calculate the dose at a particular workstation for a typical source found at that workstation.

A discrete-events processing model would then take this dose information and multiply the time in the presence of a source by the dose related to that source, and accumulate the dose over the course of the simulation to produce an integrated exposure. This method is adequate for obtaining a very approximate dose, as it accumulates dose for a personnel resource pool assuming that the only dose received by personnel resources is from the sources they are directly handling, i.e., the source at the working location for each person:

$$D_{pool} = \sum_{i=1}^{N_{exposure}} D(Source_i)\Delta t_i \quad ,$$

where dose is accumulated each time there is an exposure event up to a total of $N_{exposure}$ events (Kornreich, et al. 2002).

This is a gross approximation, especially at large material throughputs, as the more material in the room, the larger the contribution to a worker's exposure is from other sources in the room with which he is *not* working. The next step in the approximation process is to use the Pandemonium tool to create a "dose matrix," again in a preprocessing mode. This dose matrix would be composed of the dose from each source in the room at every working location in the room:

$$\begin{bmatrix} D(Source_1, \mathbf{r}_1) & \cdots & D(Source_1, \mathbf{r}_N) \\ \vdots & \ddots & \vdots \\ D(Source_N, \mathbf{r}_1) & \cdots & D(Source_N, \mathbf{r}_N) \end{bmatrix} .$$

Then, to obtain the dose for a resource pool, each time a person is in a room, i.e., each time there is an exposure event, the doses from all sources in the room at the working location are accumulated for the time the worker is in that location:

$$D_{pool} = \sum_{i=1}^{N_{exposure}} \Delta t_i \sum_{j=1}^{N_{sources}} D(Source_j, \mathbf{r}_i) \quad .$$

This approximation still assumes a static source and personnel distribution throughout the room. In actual nuclear materials operations, people move quite frequently and source items are transported occasionally. To provide as accurate an estimate of worker dose, as well as to facilitate the training of technicians (e.g., Helm and Kornreich 2002) of issues related to working in a radiation environment, we have integrated the dose modeling tool with a discrete-events simulation package such that the dose is calculated and accumulated as the simulation runs, and as people and sources move:

$$D_{pool} = \sum_{i=1}^{N_{step}} dt \sum_{j=1}^{N_{sources}} D(Source_j(t), \mathbf{r}_i(t)) \quad .$$

The key to the integration of the discrete-events model with the dose calculation kernel is the ability of the Flexsim code to support "collision spheres." Collision spheres are regions around a geometrical object such that proximity information becomes available.

As an aside, we note that the concept of dose and associated process modeling described here is easily extensible to other forms of industrial exposures, e.g., sound, heat, or airborne chemicals.

2 DOSE CALCULATION KERNEL

The dose calculated is the sum of the neutron dose and the photon (gamma) dose. In this section we briefly describe the dose calculation kernel. Flexsim™ provides the kernel with the following information:

- The total distance between the source and detector;
- The thickness and type of all shielding materials between the source and detector; and
- Source information, i.e., radius, isotopic densities, and chemical species densities.

2.1 Neutron Dose

The dose kernel calculates the neutron current density at the surface of the source and then radially attenuates it to the detector to determine the flux at the detector. The neutron current density is governed by Fick's Law, which is stated as

$$J = -D\nabla\phi \quad , \tag{1}$$

where J is the neutron current density, D is the diffusion coefficient (note this is not the dose variable mentioned previously), and ϕ is the neutron flux. The generalized neutron diffusion equation that approximates the transport of neutrons through media that contain absorbing and fissionable materials is

$$D\nabla^2\phi - \Sigma_a\phi + \nu\Sigma_f\phi + S = 0 \quad , \tag{2}$$

where Σ_a and Σ_f are the macroscopic absorption and fission cross sections, ν is the mean number of neutrons emitted per fission, and S is an inhomogeneous source term. The solution of Eq. (2) in one-dimensional radial coordinates is

$$\phi(r) = \frac{S}{B^2 D}\left[\frac{R+d}{r}\frac{\sin Br}{\sin B(R+d)} - 1\right] ,$$

where R is the radius of the source with extrapolation distance d and B^2 is the material buckling, given by

$$B^2 = \frac{\nu\Sigma_f - \Sigma_a}{D} .$$

To obtain the current at the surface (the number of neutrons leaking from the sphere per unit area), we take the derivative of the flux and multiply by the diffusion coefficient according to Eq. (1). The results of the derivation and multiplication are

$$J(R) = \frac{S(R+d)}{B^2 R^2}\frac{\sin BR - BR\cos BR}{\sin B(R+d)} .$$

Finally, we calculate the neutron flux at the detector by radially attenuating the current density to the detector position. If a is the distance from the surface of the source to the detector, the equation for the flux at the detector is

$$\phi(R+a) = J(R)\frac{R^2}{(R+a)^2} .$$

Once we have determined the flux at the detector, the neutron effective dose equivalent is determined by using standard conversion factors (ANSI/ANS-6.1.1-1991). The neutron dose is corrected for any hydrogenous shielding, which reduces the neutron energy and therefore the dose, according to a "removal" cross section of 0.15 1/cm obtained from transport calculations. The neutron dose is therefore the dose from spontaneous fission and (alpha,n) neutrons according to

$$D_n = \left[S_{sf} h_{E,sf} + S_{(\alpha,n)} h_{E,(\alpha,n)}\right]\phi(R+a)e^{-0.15\Delta} ,$$

where Δ is the total thickness of hydrogenous shielding.

2.2 Photon Dose

The photons are treated in a multi-group format; however, the calculation of the photon flux occurs on a group-by-group basis, with no inter-group interactions. The photon scalar flux is given by the solution for a self-absorbing sphere in a vacuum multiplied by a buildup factor and the attenuation obtained from shields between the source and detector. This is formally given as

$$\phi(E_j) = B(E_j)\phi\left[a, R\middle|\mu_s(E_j)\right]\prod_{i=1}^{N_{shield}} e^{-\mu_i(E_j)\Delta_i} ,$$

where
$B(E_j)$ = the photon buildup factor,
a = the source surface-to-detector distance,
$\mu_s(E_j)$ = the source photon attenuation coefficient,
$\mu_i(E_j)$ = the photon attenuation coefficient of the i^{th} shield,
Δ_i = the thickness of the i^{th} shield, and
$\phi[a,R|\mu_s(E)]$ is the unshielded flux from a self-absorbing sphere. This scalar flux is determined by an approximate solution to a double integral, which also includes the inhomogeneous photon source term. The buildup factors are calculated according to ANSI/ANS standards (ANSI/ANS-6.4.3-1991).

The photon flux at the detector is easily converted to a dose by using the ANSI/ANS fluence-to-dose factors. Summing over the energies yields the total photon dose as

$$D = \sum_{j=1}^{N_E}\phi(E_j)h_E(E_j) .$$

3 "PARTICLE" TRACING

One of most interesting and unique components of this work is the marriage of the radiation concept of particle or ray tracing with formalisms in the Flexsim™ geometric modeling tool, namely "collision spheres." The traditional sense of ray tracing involves the following of millions/billions of particles through a medium to generate transport statistics. In this case, we use a simple form of particle tracing as a means to determine the appropriate geometric parameters for calculating dose accumulated by a person (or dosimeter/detector) from a radiation source. To illustrate how this is done, consider the following example.

Given a work area with a radiation source inside a shielded glove box, two people in the area, and some other objects acting as shields (see Figure 1).

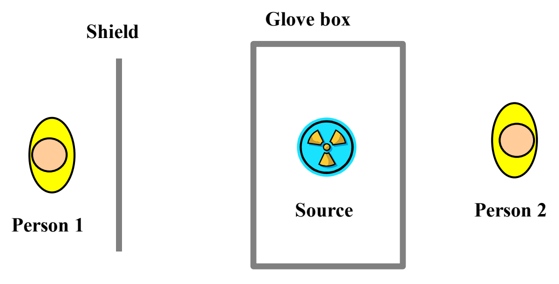

Figure 1: Particle Tracing Sample Geometry

To calculate the radiation dose that the source contributes to a person in a given time step, the following pieces of information are needed from the model:

- Source information (an attribute of the source object)
- Distance from source to person

- Type and thickness of objects (shielding) between source and person (these are attributes of each object)
- Distance from source to each shielding object between source and person.

To collect this information from the simulation model as time progresses and as objects move, a particle trace is executed at a user-defined time interval. When this happens, the source queries a table listing the unique identifier of each detector in the area. Since the source and detector (usually associated with a radiation dosimeter on a person) locations at any given time are known, the distance between them can be readily calculated. The source then "throws" an invisible particle in a straight line to each detector in turn. As the particle moves toward the person, it senses when it passes through other objects with intersecting collision spheres that are attached to each object, including particles, shields, and detectors (see Figure 2). When the particle senses a collision, the type and thickness of the object are identified and recorded as well as the distance the particle traveled to that point. Once the particle finally reaches the detector, the geometry calculation is completed since all necessary information is known. The particle trace execution is generally rapid enough to minimize impact on the overall simulation execution time.

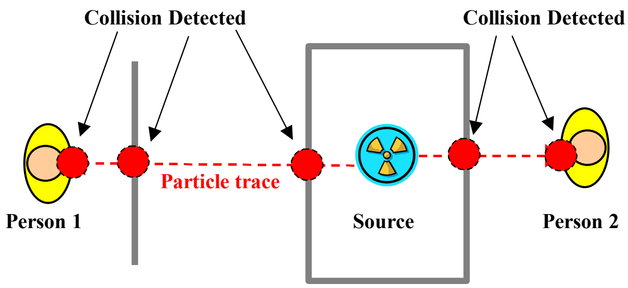

Figure 2: Particle Trace from Source to Person

4 TEST PROBLEM DEFINITION

To provide a test problem/benchmark for ultimate use in Flexsim™, we use the existing Pandemonium dose code to calculate the dose rate at specified intervals given a predetermined time-dependent situation.

In particular, we have a person (dimensions 1.5 ft × 1 ft) with a dosimeter/detector on the front of their body. The person walks parallel to the 30-ft-long hydrogenous shield of thickness 4 inches at a speed of 4 ft/s. On the other side of the shield is a plutonium oxide source, 3 ft from the path taken by the person, with characteristics as shown in Table 1. A schematic drawing of this geometry is shown in Figure 3.

We calculate the gamma and neutron (and the subsequent total) dose as measured by the dosimeter at 0.25 s intervals.

Table 1: Plutonium Source Description

Item	Value
Bulk Density (g/cm^3)	11
Mass (g)	3,000
Radius (cm)	4.2
Pu/Am Isotopic Fractions	
Pu-238	0.0005
Pu-239	0.94
Pu-240	0.055
Pu-241	0.001
Pu-242	0.0005
Am-241	0.003

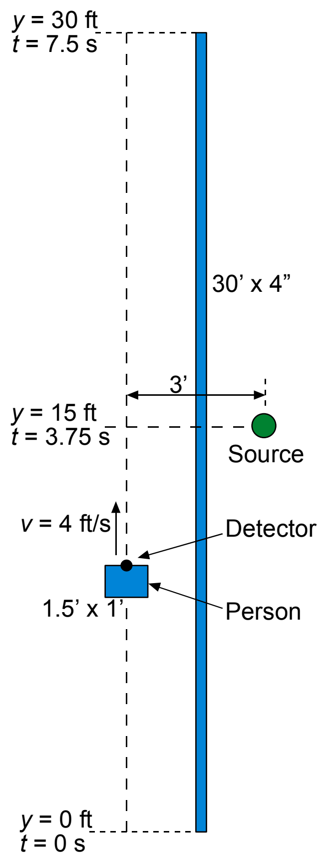

Figure 3: Test Problem Setup

We instantly see an interesting phenomenon by examining the total dose rate as a function of time, as shown in Figure 4. If we eliminate the person leaving only a "disembodied" detector moving along the path, we obtain a dose rate curve that is symmetric about the midpoint in the path (y = 15 ft, t = 3.5 s), as expected. However, when the person is in position as shown in Figure 3, initially there is only the long hydrogenous shield between the source and detector. Upon reaching the midpoint of the path and thereafter, portions the person are between the source and detector that is located on the front of the person.

In Figure 4, we note two discontinuities in the curve with the person in place (the blue curve). The first discontinuity is at the midpoint where at $t = 3.5 - \varepsilon$ s, the only shield between the source and detector is the long hydrogenous shield, and at $t = 3.5 + \varepsilon$ s, there is suddenly the long hydrogenous shield plus ~ half of the width of a person between the source and detector. This results in a true discontinuity in the dose rate curve. After the midway point, as the person moves away from the source, the ray tracing through the person result in an increase in the hydrogenous shield thickness until the line between the source and detector reaches the lower righthand corner of the person, where the shielding thickness is the greatest. As the person moves farther away, the shielding from his body decreases. The result of this ray tracing formalism is a discontinuity in the slope of the dose rate around $t = 4.75$ s. This slope discontinuity is clearly the result of modeling a person's body as a rectangular form. Were we to model it as an ellipse for example, there would be changes in slope, but the discontinuity would not exist.

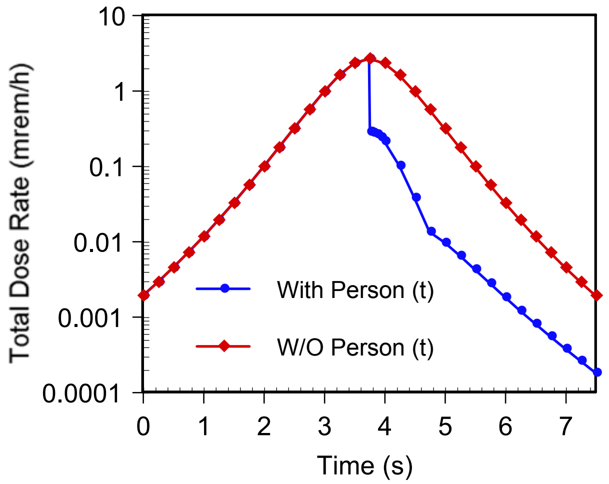

Figure 4: Test Problem Total Dose Rate Versus Time

Clearly, the shielding of detectors by the bodies of workers is an interesting an important phenomenon to quantify. In a nuclear facility, the worker dose that is most generally associated with regulatory limitations is his whole body dose, or the dose determined from the dosimeter/detector on the front of his body. However, if we examine the cumulative dose, as in Figure 5, we note that the dose measured by the detector is approximately twice as large without the person "self-shielding" as if the person is there.

In this case, and in reality, we have competing effects in action. First, the potential of a person to act as a shield is evident, and it may reduce the dose measured by the dosimeter below what is actually received by the persons body. However, when the person is facing away from a source, the ionizing radiation is first encountering the back of the person, which is generally composed of bone and thick muscles. Muscle is much less susceptible to damage than organs, which is why dosimeters are worn on the front

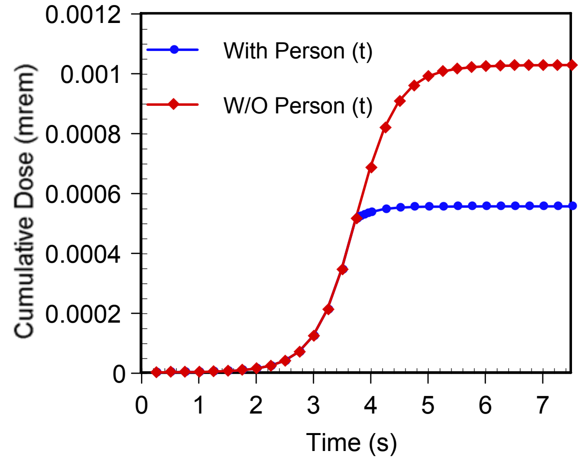

Figure 5: Test Problem Cumulative Dose Versus Time

of the body, where there is less shielding of the organs in the chest and abdominal areas.

Where the above phenomena become important, especially as related to a process model such as might be constructed in Flexsim™, is in the complex operations of a real nuclear facility. When there are several sources and persons in a room, simply modeling the dose a person receives from his source may significantly underestimate the dose they will receive. When the room is active, there is a very complex interaction of sources and shields, *including persons*, such that the marriage of a dose tool like Pandemonium with a process model like Flexsim™ becomes immensely valuable. In the test problem, the shielding of the detector by the person may be less important because much of the dose is being received by his back, but if he is acting as a shield to another person, this significantly could reduce the dose to the second person. The ability to calculate and demonstrate this phenomenon is one of the key reasons for "arranging" this marriage.

5 FLEXSIM™ RESULTS

To test the ability of the discrete-events code Flexsim™ to support dose calculations, we create a model of the test problem in this software package. Figure 6 contains a Flexsim™ 3D visualization of the test problem setup shown in plan view in Figure 3. Flexsim™ calculates the thickness of the hydrogenous shielding, which is then used by the dose calculating kernel (currently a post-processing calculation) to obtain the dose to the worker.

In the model execution, Flexsim™ "throws" a photon from the source icon toward the detector. The distance from the source to the detector minus the shield wall thickness gives the thickness of air through which the radiation passes. If the photon collides with the person's collision sphere, it is noted that the person has been intersected.

As discussed previously, there is a nuance in the way Pandemonium calculates the hydrogenous shielding

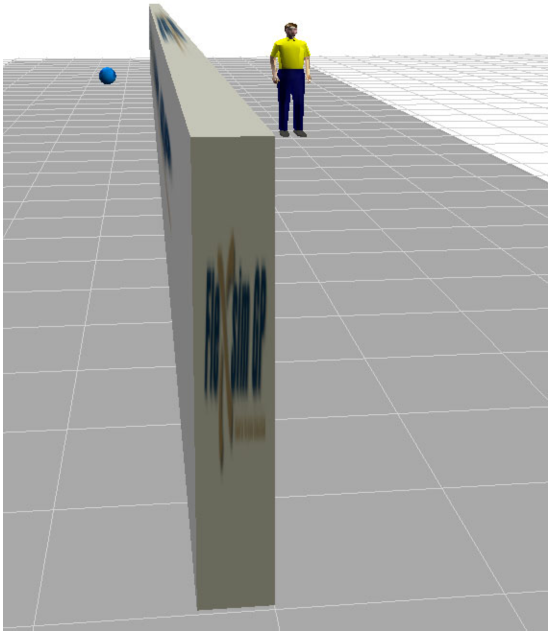

Figure 6: Test Problem Setup – Flexsim™

thickness, i.e., it models a person as a rectangular solid and calculates the exact thickness of hydrogenous material traversed. Flexsim™ does not model the person in this fashion. For the Flexsim™ calculations, we model the thickness of the hydrogenous shielding according to

$$\Delta_H = \frac{4''}{\cos\theta} + 9''(\text{when collide}) \quad . \qquad (3)$$

In Eq. (3), the first term is an exact representation of the thickness of the hydrogenous shield wall as a function of time, were the angle is time-varying. The second term is a gross approximation to the thickness of hydrogenous shielding that comes from the person's body being between the source and detector. The thickness 9 inches is the horizontal half-thickness of the person. In general, Eq. (3) will underestimate the amount of hydrogenous shielding presented by the person.

In Fig. 7, we show the dose rate results as a function of time for the Flexsim™ calculations. Note that before the person crosses the midway point of his trajectory, the agreement is exact, as expected. After the midpoint, Flexsim™ slightly underestimates the shielding (note the scale is logarithmic) and therefore overestimates the dose rate. In like fashion, we see a similar phenomenon in the cumulative dose as a function of time (see Figure 8), where Flexsim™ overestimates the cumulative dose by about 15%.

6 SUMMARY

This paper demonstrates the first step in a fully-integrated process model with dose calculation capability. The process model, which was constructed in Flexsim™, calculates the shielding distances for a test problem, which is one of the key components of a dose calculation. The key facilitating capability in Flexsim™ is that of "collision spheres," where we are able to determine when objects are encountered by interrogative particles, or particle ray traces, that are constructed in the model. Future work could include a more accurate determination of the person's shielding thickness as well as a different means of calculating the thickness of the shielding wall. One possible mechanism is to overlay the wall with a series of collision spheres such that the ray tracing particle determines the wall thickness according to the number of collision spheres it encountered. Of course, another logical extension of this work is to include the dose calculating algorithm directly in Flexsim™.

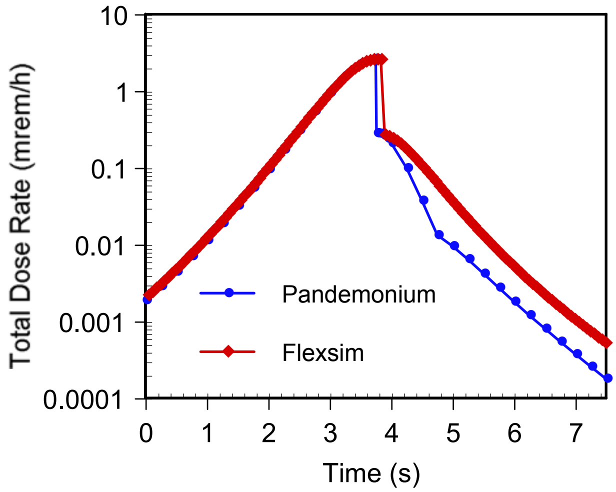

Figure 7: Test Problem-Pandemonium v. Flexsim

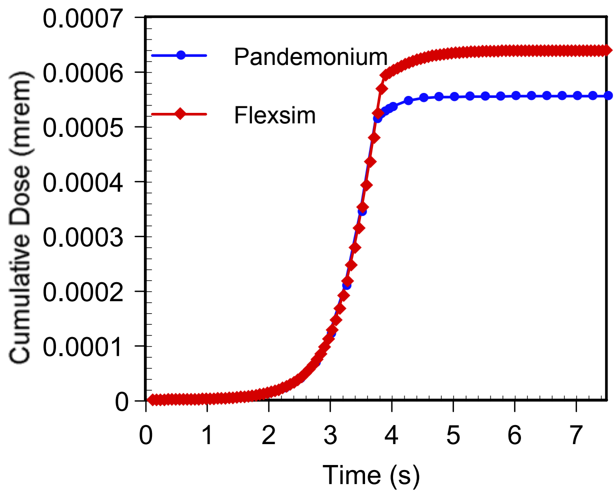

Figure 8: Test Problem Cumulative Dose Versus Time

ACKNOWLEDGMENTS

LA-UR-04-2614

REFERENCES

American National Standard for Neutron and Gamma-Ray Fluence-to-Dose Factors, 1991. ANSI/ANS-6.1.1-1991, American Nuclear Society.

American National Standard for Gamma-Ray Attenuation Coefficients and Buildup Factors for Engineering Materials, 1991. ANSI/ANS-6.4.3-1991, American Nuclear Society.

Helm, T. M. and D. E. Kornreich. 2002. Visualization of a Changing Dose Field, In *2002 Advanced Simulation Technologies Conference*, San Diego, California.

Kornreich, D. E. and D. E. Dooley. 1999. A Two-Dimensional Point-Kernel Model for Dose Calculations in a Glovebox Array, *Transactions of the American Nuclear Society*, **81**, 249.

Kornreich, D. E., J. W. Jackson, S. T. Boerigter, W. A. Averill, and J. H. Fasel. 2002. Dose Estimates of Alternative Plutonium Pyrochemical Processes, In *Proceedings of the 12th Biennial Radiation Protection and Shielding Division Topical Meeting*, Santa Fe, New Mexico.

AUTHOR BIOGRAPHIES

GEORGE TOMPKINS is a Technical Staff Member in the Systems Planning and Analysis Group at Los Alamos. His interests include output analysis and agent modeling techniques. Before coming to Los Alamos he was a consultant for SAS Institute Inc. He received a Ph.D. in Industrial Engineering from Kansas State University.

DREW E. KORNREICH is a Technical Staff Member in the Systems Planning and Analysis Group at Los Alamos. He holds a Ph.D. in Nuclear Engineering from the University of Arizona, with interests in criticality safety and neutral particle transport theory. Recent work at Los Alamos includes semi-analytical benchmarking and process dose modeling.

ROBERT Y. PARKER is a Technical Staff Member in the Systems Planning and Analysis Group at Los Alamos. He received his Bachelor's and Master's degrees in Mechanical Engineering and Manufacturing Engineering from Brigham Young University. He has been actively involved in simulation modeling and analysis of industrial and nuclear-related systems for the past 11 years.

ANDREW KOEHLER is a technical staff member in the Statistical Sciences group at Los Alamos. His research focuses on systems analysis, computer simulation, and decision making in the operation of hazardous technical systems. He holds a Ph.D. from UC Berkeley's Goldman School of Public Policy. Before coming to Los Alamos, he was a researcher at UC Berkeley's Center for Nuclear and Toxic Waste Management.

JOHNELL GONZALES-LUJAN is a Technical Staff Member in the Systems Planning and Analysis Group at Los Alamos. Since joining the Lab in 1992, she has performed systems analysis of material processing and manufacturing operations for defense and commercial applications. She received her Masters of Business Administration in Operations Research and Management Science and her Bachelors of Business Administration in Business Computer Systems from the University of New Mexico. She is currently a member of INFORMS, IIE, and APICS.

ROBERT BURNSIDE is a Technical Staff Member in the Systems Planning and Analysis Group at Los Alamos. His current interests are in modeling fabrication and process lines. Since coming to Los Alamos, he has been involved with developing simulation models of the defense production process. He received his Masters in Nuclear Engineering from Carnegie-Mellon University and a Masters of Business Administration from the University of Washington.