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Hot Cell Facility Criticality Safety Assessment for Storage of Medical Isotope Targets and Process Waste

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Abstract

An assessment of the potential criticality hazard associated with isotope processing operations in the Hot Cell Facility has been accomplished in accordance with DOE-STD-3007-93. This assessment includes the consideration of the quantities, forms, and locations of fissile material that will exist in the HCF. Contingency analyses have been accomplished to evaluate the multiple events which could potentially result in a criticality event. These analyses included the effects of flooding and procedural errors. Validated calculational techniques have been used to evaluate all credible configurations of fissile material. A wide range of fissile arrays and hypothetical configurations were numerically analyzed to assess the potential for criticality. In all cases, the results indicated that fissile material arrays would remain subcritical in the HCF. The design features and administrative controls on which these analyses were based are identified.

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1.0 Introduction

The Hot Cell Facility (HCF), with a principal mission of isotope processing, will be used to process and store fissile materials in sufficient quantity to require a formal evaluation of criticality issues. This Criticality Safety Assessment (CSA) describes the types, forms, inventories and locations of fissionable (or fissile) materials that may be present within the facility. It also provides analyses to support the conclusion that the fissile materials used for isotope production will remain subcritical under all normal, abnormal, and accident conditions.

The HCF is described in the Safety Analysis Report (SAR) (Mitchell, et al., 2000). A layout of the facility is shown in Figure 1. The HCF will receive, process, and store fissile materials used for isotope production. The materials will enter the HCF in the form of "targets," which will either be stored or processed. Unirradiated targets will be stored in storage safes located in Rooms 108, 112, 113, or 113A. Irradiated targets will be removed from shielded casks inside Zone 2A, and will be processed within Zone 2A. Residual waste containing fissile materials will be temporarily staged in Zone 2A prior to movement into Room 109 for longer storage prior to off-site shipment.

2.0 Description

The HCF will receive, process and store fissile materials, principally in the form of uranium dioxide (UO_2) enriched to 93% ^{235}U . Normally, this material will be brought into the HCF as part of isotope production "targets," which are stainless steel tubes internally coated with 25 to 35 grams of UO_2 . Irradiated targets will be processed in steel confinement boxes (SCB's) also identified as ventilation Zone 1. The configuration of these SCB's inside Zone 2A is shown in Figure 2. During processing, the UO_2 is dissolved in acid and isotopes are chemically extracted. Following processing, the UO_2 solution will be solidified in stainless steel waste containers as a concrete mixture. While only one target is processed at a time in each SCB, several targets or their contents may be present in each process box. Space limitations, the potential for window radiation damage, process cleanliness requirements, and Technical Safety Requirement (TSR) administrative limits will all constrain the number of targets that will be permitted in a process box at any time. Normally, the waste residue containing the fissile ^{235}U will be removed from the SCB's on a daily basis. The residual waste materials will be stored temporarily in barrels in Zone 2A (in the elevator pit), and then transferred into the waste storage area, Room 109, on carts, each of which holds either 4 or 8 barrels of waste. The storage configuration in Room 109 is depicted in Figure 3. To meet Department of Transportation (DOT) requirements for off-site shipment of waste, the ^{235}U content of each barrel will be administratively limited. Additionally, the volume of the barrel and the volume of the process waste will physically limit the amount of fissile material which can be placed in a barrel. Eventually, the waste barrels will be removed from Room 109 through Room 108 for packaging and shipment to the Nevada Test Site for disposal. Room 109 will have storage capacity for 180 barrels of waste. To accommodate production operations with intermittent shipments and the potential for disposal shipment delays, the storage space will normally not be allowed to be totally filled. Additionally, to remain within Special Nuclear Material (SNM) administrative limitations for Category III material as defined by DOE M 474.1-1A, the total ^{235}U inventory in Room 109 will be administratively limited.

Unirradiated targets may be brought into the HCF for examination or storage. Routine storage of targets will be in standard 2 or 4 drawer security safes. Small numbers of targets may be present in any region of the HCF, but the number of targets at any single location will be limited so as to preclude criticality. Other fissile materials which may be brought into the HCF for temporary examination or storage will be examined on a case-by-case basis for criticality compatibility with the isotope production inventory, and a separate criticality analysis will be accomplished.

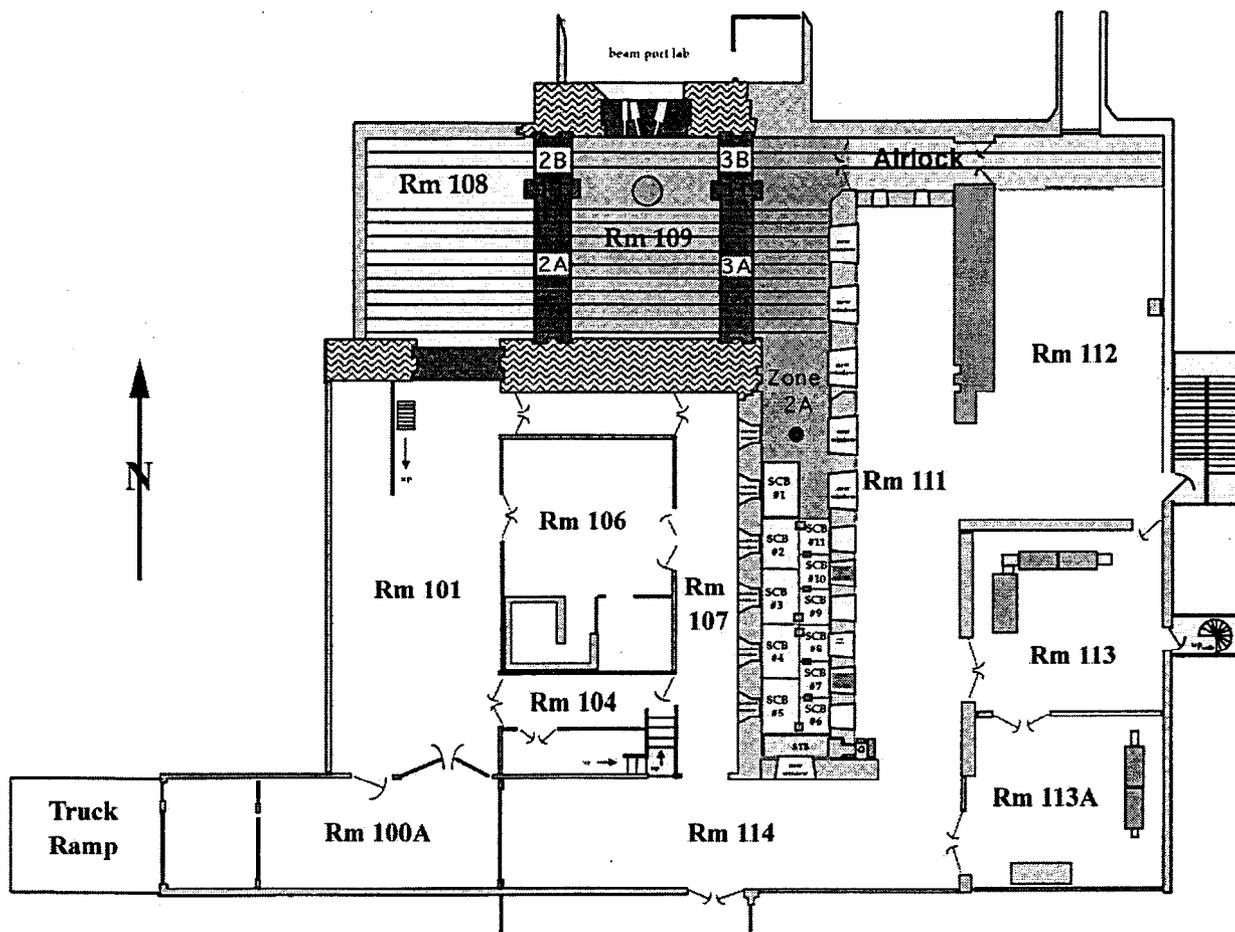


Figure 1. HCF Layout.

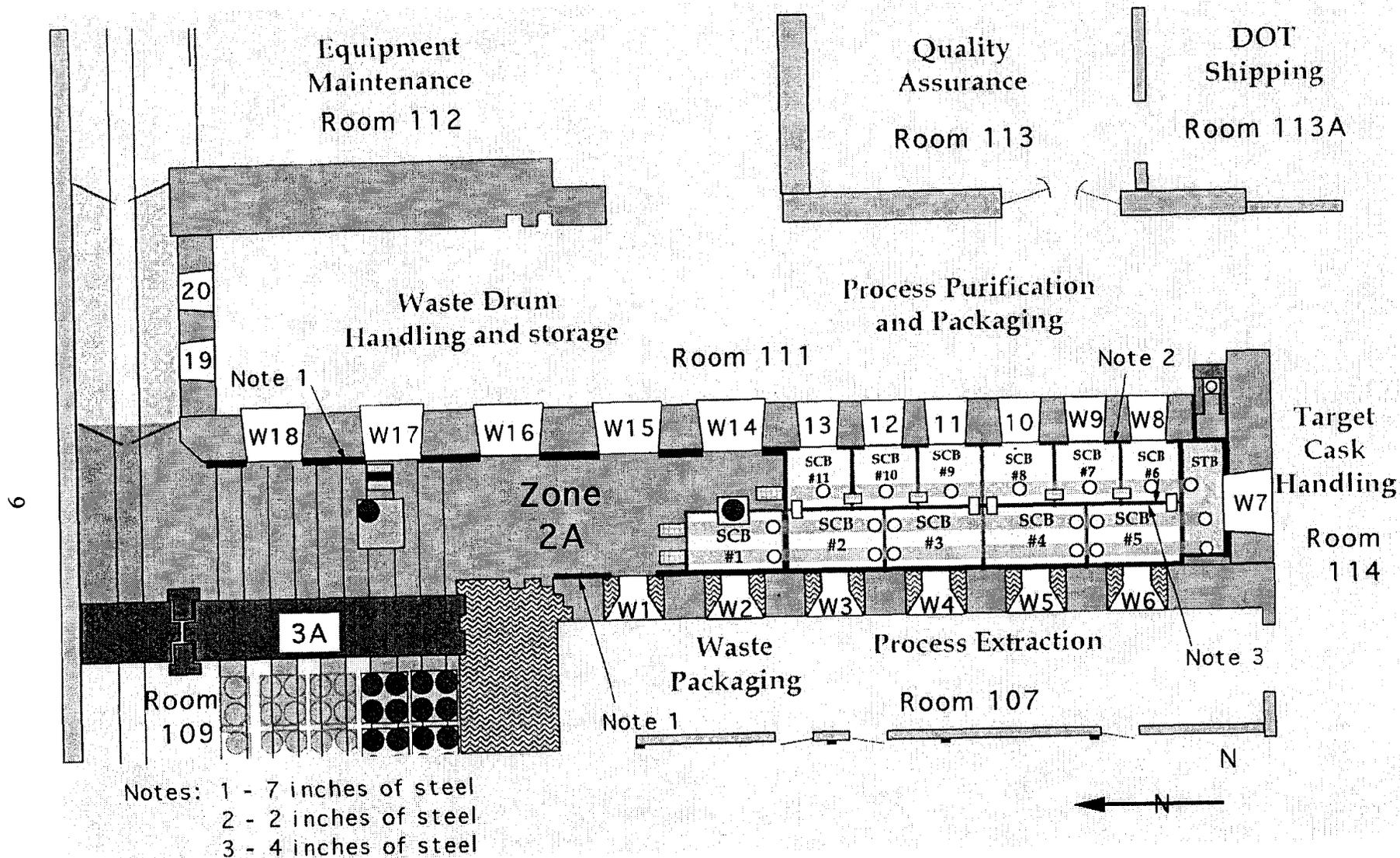


Figure 2. HCF SCB Layout.

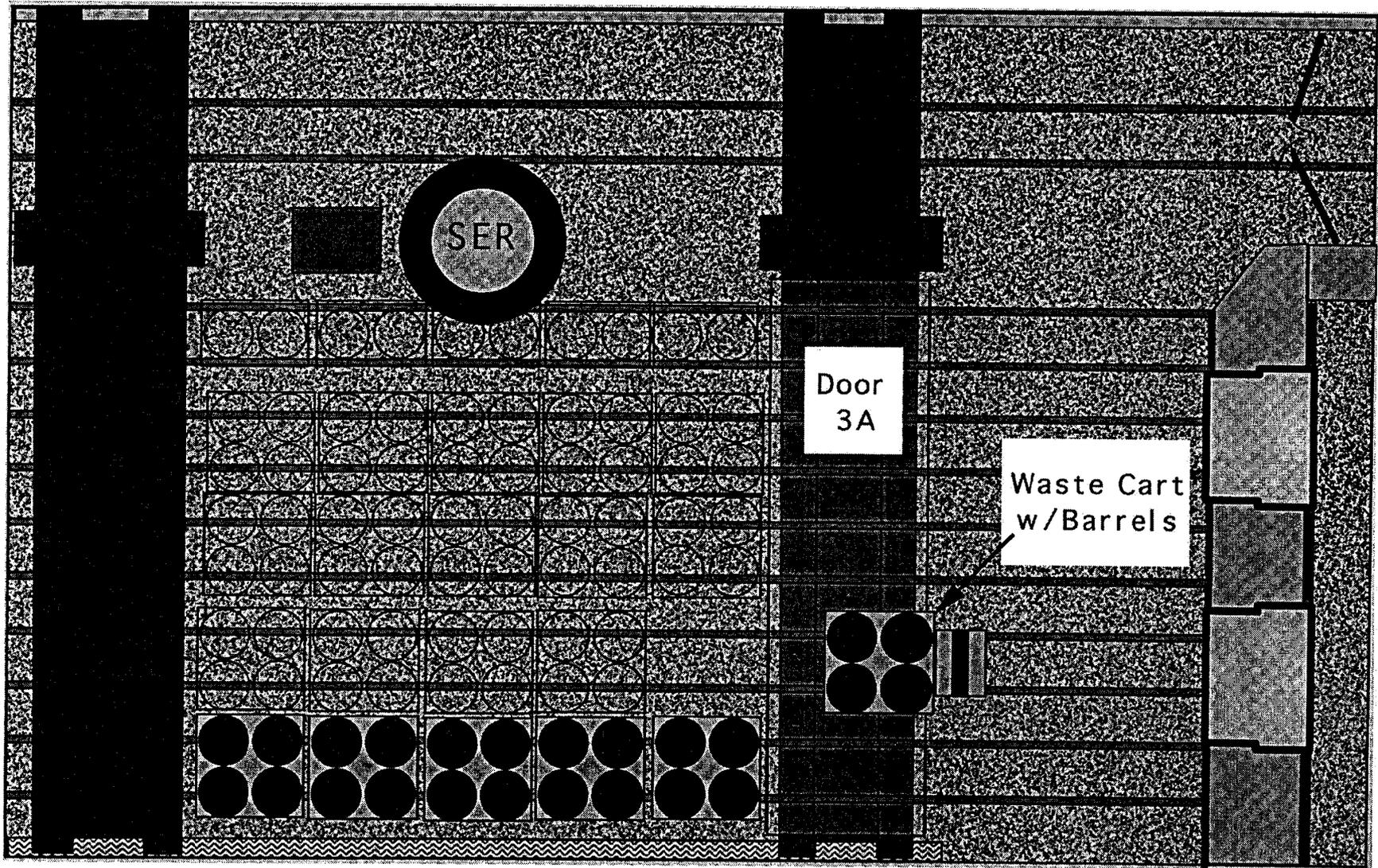


Figure 3. Room 109.

The HCF has several areas in which the potential for an inadvertent criticality exists. These are the SCBs, the Zone 2A processing canyon, Rooms 108, 109, 110, 112, 113, 113A and the HCF east (monorail) storage holes. Chapter 2 of the HCF SAR describes each of these areas in detail, including facility and equipment drawings.

3.0 Requirements Documentation

The pertinent criticality-safety requirements for nuclear criticality safety in the HCF are described in the Sandia National Laboratories (SNL) Environmental Safety & Health (ES&H) Manual, Supplement GN470072, "Nuclear Criticality Safety" (Philbin, 1998). This manual addresses the requirements in all applicable DOE Orders such as 5480.21, 5480.23, 420.1, and ANSI standards. It also includes the basis for criticality requirements, record keeping, assessments for potential criticality events, criticality safety control parameters, conducting criticality safety analyses, preparation of plans and procedures, requirements for criticality alarms, personnel training, posting, and operational considerations. The Supplement requires that a facility Criticality Safety Assessment (CSA) be prepared in accordance with DOE-STD-3007-93.

4.0 Methodology

The safety of planned configurations of fissile material in the HCF has been examined by validated calculational techniques. Los Alamos National Laboratory's MCNP (Monte Carlo N Particle) code, (Briesmeister, 1993) Version 4A, running on a Dell OptiPlex GXMT5133 (Intel Pentium) operating under MS-DOS Windows NT Version 3.51, using ENDF/B-IV cross sections, was used to examine potential fissile configurations (Romero, 1998a). MCNP is one of many neutron transport simulation codes commonly used in criticality analyses to model complex geometries as closely as possible while simulating their neutronic behavior with the Monte Carlo method.

A number of benchmark calculations using MCNP version 4a and input decks from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) were accomplished by Bodette and Harms (Bodette, 1996). These calculations included a variety of fissile compositions and configurations. The configurations relevant to the Hot Cell Facility (HCF) Criticality Safety Assessment (CSA) include a highly enriched unmoderate assembly (Godiva) and an intermediate energy heterogeneous uranium dioxide system (TOPAZ) flooded with water. The results of these benchmarks are as follows:

System	True K_{eff}	ICSBEP Value	SNL MCNP Result
Godiva	1.000±0.001	0.9968±0.0009	0.99683±0.00086
TOPAZ	1.000	0.9971±0.0008	0.99685±0.00084

These results indicate that SNL computations underestimate k_{eff} by 0.0032 for these fissile configurations. The largest bias for other fissile configurations reported by Bodette and Harms in the benchmark analysis was 0.005.

Additionally, this version of MCNP has been used to model a number of configurations of the Annular Core Research Reactor, with good agreement between calculated results and measured operational characteristics. Additional calculations were performed using KENO.Va (Miles, 1985) and Hansen-Roach cross sections, by (Vernon, 1998), which compared favorably to results obtained with MCNP on identical configurations (Romero, 1998b).

A text-input file is used in MCNP to describe the geometry and material composition of the model. The input file is divided into three major sections: cell cards, surface cards, and material cards. Cell cards group together surfaces (e.g. cylinder, planes, etc.) to form cells or regions. Material cards define the materials contained in each cell of the geometry and their composition. A material mixture is described by entering the weight fraction or atom density of each constituent. The material cards define the locations of the fission source points and specify how many neutron generations will be simulated in each computer run. An output file is produced after the entire calculation is completed with a final numerical value for k_{eff} and its associated standard deviation. A sample copy of an input and output file for a modeled scenario from the criticality evaluations performed for this CSA are attached in Appendices A and B, respectively. In addition, a sample calculation detailing the process used to determine the necessary atom densities of the UO_2 region of the target, and the ^{235}U - H_2O mixture in waste storage evaluations is included in Appendix C.

5.0 Discussion of Contingencies

Processing of isotope targets is rigorously governed by procedure. Processing areas are required to be maintained in a neat and clean condition to meet Food and Drug Administration (FDA) and Good Manufacturing Practices (GMP) guidelines. Process throughput will require that material flow through the HCF not be restricted and allowed to accumulate at any point, or it will constrain follow on-production, preventing the further accumulation of fissile material. Furthermore, such accumulation would be readily apparent and will be monitored on a near continuous basis during production operations. A maximum expected processing rate of 6 targets per day in the HCF limits the quantity of material at risk of criticality at any one time to about one-fourth of that established as an inherently safe mass of 700 g. ^{235}U by GN470072. Multiple, independent errors in process control would be required to permit accumulations which would result in a critical configuration. Further, errors would need to occur repeatedly over multiple days, and would have to go unnoticed in a rigorous production environment.

Based on results of evaluations described below, and taking into account the number and magnitude of errors which would be required, the likelihood of a criticality accident in the HCF is considered to be incredible, or less than a probability of occurrence of one in one million per year. With this assessment, formal contingency analyses are not required in accordance with DOE-STD-3007-93. Nonetheless, contingency analyses have been performed and are described below to provide substantiation of the basis for these conclusions.

One of the key aspects of this criticality assessment is that substantial moderation is required to achieve significant neutron multiplication for the quantities and form of fissile materials which will be present in the HCF. Thus, the likelihood of the presence of substantial quantities of water or other hydrogenous material is a key element in the assessment of the potential for criticality.

Flooding of the HCF due to natural phenomena has been established as a beyond the design basis of the facility event based on: the location of the facility; contour of surrounding terrain; proximity to natural bodies of water; and the degree of rainfall required to result in surface runoff. Flooding of the HCF due to fire suppression efforts which would be of sufficient magnitude to be a factor in criticality analysis is not credible. The quantity of flammable materials in the HCF is administratively limited. The amount of water which might be used to suppress a fire, either by an automatic system or a manned response, would be proportional to the amount of flammable material available for combustion. The volume of the HCF to a depth of 1.8 meters (6 feet, sufficient to inundate a safe) is approximately 2800 m³ (100,000 ft³ or 700,000 gallons), which includes a volume of about 370 m³ represented by the catacombs. The use of this volume of water to suppress a limited fire in the HCF is not reasonable. The only remaining potential for flooding of the HCF is due to a break in utility water supply lines. If a break were induced by human interaction, a response to shutoff the flow of water would preclude the buildup of water to significant levels. For a significant buildup to occur, the water line break would have to go undetected, which implies that the HCF was not occupied. The likelihood of such a spontaneous break in the lines is extremely low, but not beyond the bounds which should be considered in these assessments.

Thus, despite the extremely low likelihood of flooding in the HCF, the effects of such flooding on arrays of fissile material have been evaluated. In all cases evaluated, dry arrays of fissile material are highly subcritical. Considerable water moderation is required to achieve significant neutron multiplication with Cintichem Targets, and all credible flooded configurations remain subcritical. The following tables provide an evaluation of events which would be required to occur concurrently before a criticality accident could be possible in four separate scenarios: target storage; target processing; waste handling; and waste storage.

Contingencies for Storage Criticality:

Event No.	Event Description	Barriers to Event Occurrence
1	Excessive ²³⁵ U placed in Safe	Rigorous QC on target manufacture and acceptance; Volume of Safe and target
2	Internal and external flooding	Open HCF configuration allowing water flow, Volume of HCF; External event flood is beyond design basis; limited fire fighting water requirements; Target tube will preclude internal flooding

Evaluations of storage configurations and the degree of flooding required to achieve criticality are described in Section 6.

Contingencies for SCB Criticality:

Event No.	Event Description	Barriers to Event Occurrence
1	Excessive quantity of ^{235}U placed in single SCB	Rigorous QC on target manufacture and acceptance for processing; SCB Administrative limits; multiple successive physical actions required to introduce targets into SCB; Radiation damage to windows, resulting in browning which prevents further operations;
2	Event 1 occurs over multiple days	SCB cleanup each day
3	SCB Flooding	Limited availability of water and other hydrogenous materials; SCB administrative limits; SCB cleanup each day

SCB's fissile content is administratively limited to an inherently safe mass (350 g ^{235}U), which would represent about 12 maximally loaded targets. Only a single target can be brought into Zone 2A and introduced into the SCB at a time.

Contingencies for Waste Handling (Zone 2A) Criticality:

Event No.	Event Description	Barriers to Event Occurrence
1-N, where N represents number of excessively loaded targets	Barrels loaded with excess ^{235}U	Rigorous QC on target manufacture and acceptance for processing; Process Chemistry limits UO_2 dissolution; Barrel volume; Barrel Administrative limits (DOT Based); operator training & procedures; multiple successive failures required
N+1	Zone 2A (Elevator Pit) Flooding	No source of water in Zone 2A; HCF Volume

Evaluations for waste barrel criticality are based on waste storage evaluations for Room 109, which are described in Section 6.

Contingencies for Waste Storage (Room 109) Criticality:

Event No.	Event Description	Barriers to Event Occurrence
1-N, where N represents the number of excessively loaded targets	Multiple barrels loaded with excess ^{235}U	Rigorous QC on target manufacture and acceptance for processing; Process Chemistry limits UO_2 dissolution; Barrel volume; Barrel Administrative limits (DOT Based); Room 109 Administrative Limits; operator training & procedures; multiple failures required
N+1	Flooding of Room 109	No source of water in Rm. 109; HCF Volume; Leakage into Catacombs

Criticality evaluations of waste storage configurations, including the effects of excess ^{235}U mass, and the degree of flooding required to achieve criticality are described in Section 6.

As described previously, the processing of isotope production targets is rigorously governed by procedure and by Good Manufacturing Practices (GMP), and the unintended accumulation of fissile material is not consistent with a production operation. Multiple, independent errors in process control would be required to permit accumulations which would result in a criticality accident. Furthermore, errors would need to occur repeatedly over multiple days, and would have to go unnoticed in a rigorous production environment. As described in the evaluations which follow, the multiple process parameters that will limit accumulation of fissile materials and preclude criticality in the HCF include:

- Target ^{235}U content.
- Number of targets and ^{235}U mass in storage configuration.
- Geometry of storage configuration.
- Number of targets/ ^{235}U mass simultaneously in-process.
- Availability of moderating materials.
- Daily disposition of residual waste.
- Waste form.
- Waste storage configuration (geometry).

Based on the evaluations accomplished in this CSA, it is considered incredible that the multiple independent errors in these process parameters required to achieve inadvertent criticality could occur without detection and corrective action. With this assessment, the double contingency principle, as stated in DOE O 420.1, is met in the HCF.

6.0 Evaluation and Results

6.1 Introduction

Several analyses, using validated computational methods, have been completed to evaluate the storage of medical isotope targets and associated process waste (Romero, 1998a-e). These analyses include normal and abnormal storage configurations, and include evaluations of the effects of flooding. Most fissile material in the HCF will enter the facility as targets which contain ^{235}U in the form of UO_2 coated on the internal stainless steel wall. These targets will be either stored or processed. Storage locations may exist throughout the HCF, however processing is limited to Zone 2A, which is heavily shielded. Following processing, the waste is solidified in concrete and is stored first in Zone 2A and then moved into Room 109. Based on this process flow, the following configurations were evaluated for criticality:

1. Storage of unirradiated targets in a safe.
2. Processing of irradiated targets in process boxes.
3. Temporary storage of process waste in Zone 2A.
4. Interim storage of process waste in Room 109.

As described in Section 4, Los Alamos National Laboratory's MCNP (Monte Carlo N Particle) code, (Version 4A) and KENO.Va were used to accomplish these evaluations. MCNP is one of

many neutron transport simulation codes commonly used in criticality analyses, and this code has been extensively used to assess criticality at SNL Technical Area V (TAV).

6.2 Model Descriptions

There were two reasons why ^{238}U was not considered in the ^{235}U - H_2O mixture in any of the modeled waste storage configurations:

1. Even though some burn-up had occurred for all processed targets with some uncertainty in the exact ratio between ^{235}U and ^{238}U , it was assumed that the mixture remained highly enriched in ^{235}U ; and,
2. Without having to justify the amount of ^{238}U present, we defaulted to a more conservative k_{eff} by not introducing additional parasitic absorption caused by the addition of ^{238}U .

6.2.1 Target Description

A Cintichem target is a stainless steel, hollow tube 3.18 cm (1.25 in.) in diameter and 45.72 cm (18.0 in.) in length (Miller, 1996). The thickness of the stainless steel tube is nominally .075 to .089 cm (.03 to .035 in.), but was modeled at 0.0635 cm thick (.025 in.). This is approximately 240 grams of stainless steel, which is the lower acceptability limit for fabrication of the target. Fissile material mass loadings of 30 grams of ^{235}U were evaluated, which is 50% greater than the current nominal target loading. This evaluation was accomplished to encompass future expectations to increase target ^{235}U loading. The length of the UO_2 coating is modeled as 41.9 cm (16.5 in.). A radial and axial view of the target as modeled in MCNP is shown in Figure 4, and an axial cross-sectional view of the MCNP modeled target as compared to the nominal Cintichem target is shown in Figure 5.

A major difference between the target as modeled for MCNP and the actual target is the omission of the top and bottom stainless steel end caps. The end caps were omitted from the model to keep the description of the model relatively simple yet detailed enough to simulate a realistic geometry. Additionally, this should conservatively bias the results, since additional stainless steel, which acts as a neutron absorber, will reduce the effective multiplication.

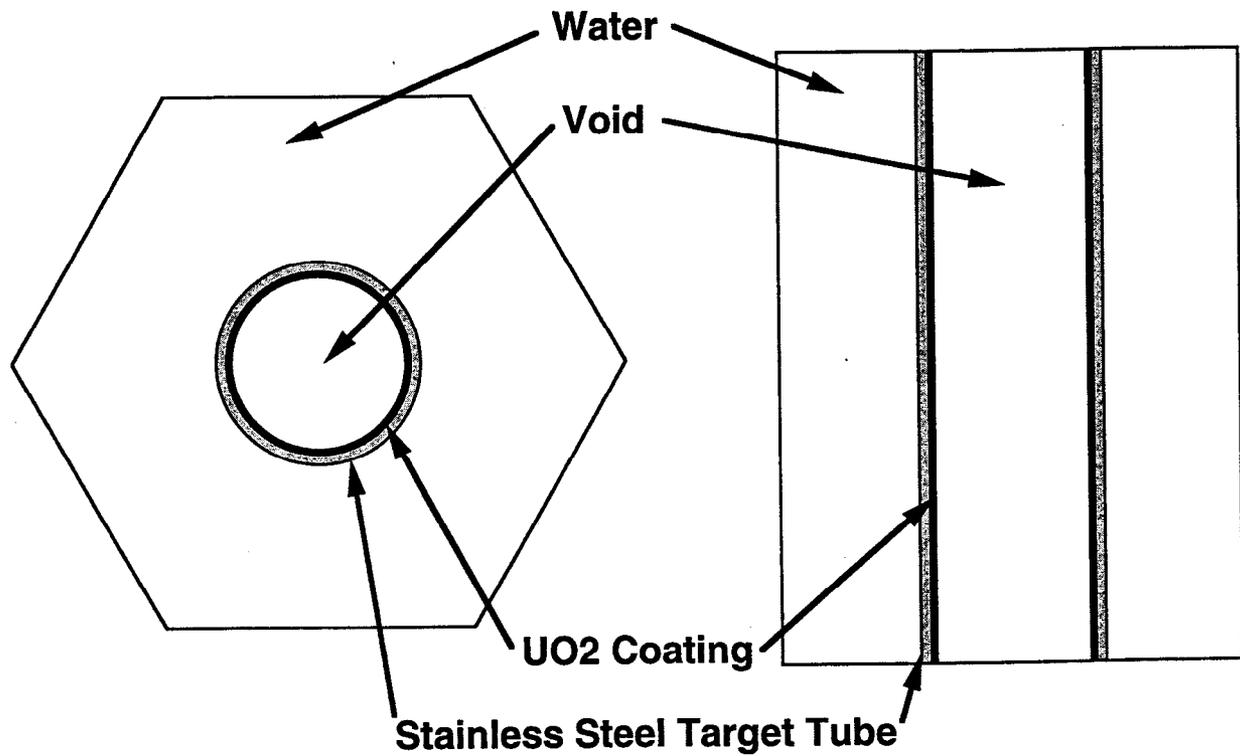


Figure 4. Radial and Axial Views of MCNP Target Model.

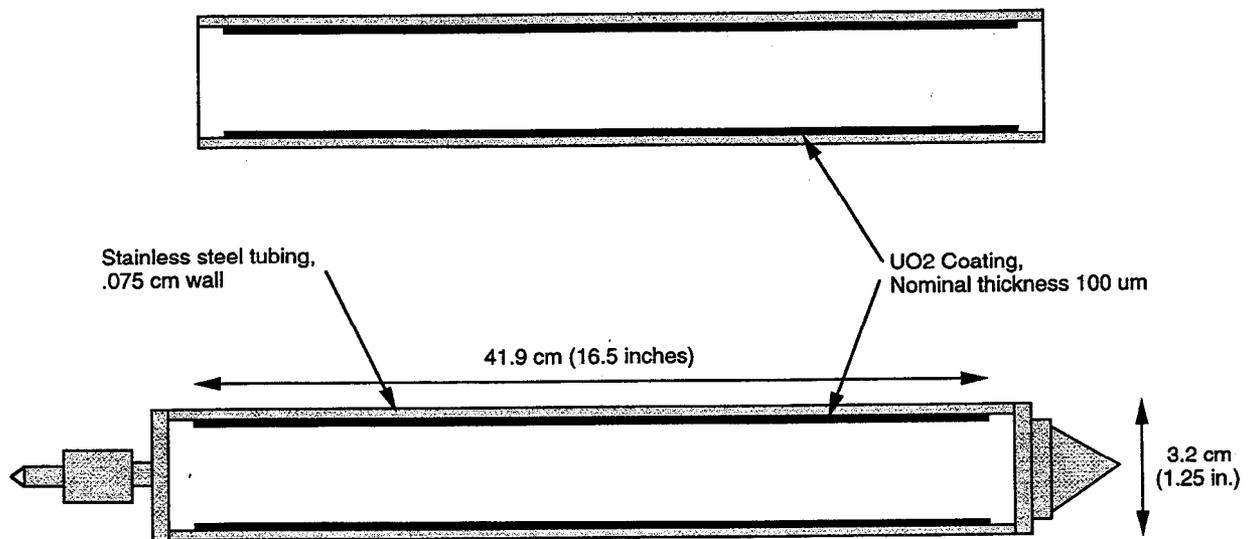


Figure 5. MCNP and Target Configurations (not to scale).

6.2.2 Target Storage Configurations

Unirradiated targets will be stored in a standard four-drawer safe in the HCF. This configuration was modeled by arranging the targets in four groupings representing the safe drawers. Each drawer has internal dimensions of 25.4 cm (10 in.) high, 38 cm (15 in.) wide, and 45.72 cm (18 in.) deep, with 33 cm (13 in.) drawer to drawer spacing. The targets are modeled in a hexagonal close packed lattice with a triangular pitch of 3.2-cm (1.25 in.). For this pitch, 88 targets will fit in each drawer in 9 layers as depicted in Figure 6, for a total of 352 targets in the safe.

Configurations of 79 and 69 targets per drawer at a pitch of 3.2 cm were also evaluated to ascertain the reactivity effect of partially filled drawers (i.e. 8 layers of targets would total 79 and 7 layers of targets would total 69). The space between each drawer of targets is modeled as filled with water for flooded configurations, even though the material separating each safe drawer would prevent water from occupying this entire region.

To evaluate the abnormal condition which might exist with dispersed targets in partially loaded drawers, analyses have been performed for targets at a pitch greater than the nominal 3.2 cm. These analyses were based on an array of targets in a volume of 36 x 102 x 46 cm, which represents the volume of four safe drawers. The targets were spaced at a pitch of 4.5 cm, based on previous calculations (Parma, 1997) which indicated that this pitch produced near-optimum neutron multiplication for an array of internally dry targets (Romero, 1998c). This pitch will accommodate 156 targets in the above volume, as depicted in Figure 7. The representation of the analyzed array yields results with greater neutron multiplication than that which would exist for the actual storage volume of 36 x 124 x 46 cm. Although there is no credible physical mechanism to achieve an average target pitch of 4.5 cm in a HCF storage configuration, this evaluation was performed to assess the effect for accident induced geometry changes. It should also be noted that if more than 39 targets are stored in each drawer, this pitch is not realizable.

6.2.3 Waste Storage Configurations

Process waste from each target will be solidified in concrete inside a stainless steel container 15 cm (6 in.) in diameter and 7.5 cm (3 in.) high, having a total volume of about 1.3 liters.

Somewhat less than 300 ml of process solution is solidified with an approximate equal volume of concrete inside this container, as represented in Figure 8. Waste containers with solidified waste will be removed from processing stations at the completion of each shift and will be moved to SCB1 where they, along with associated process waste (syringes, empty target shells and other hardware), will be placed in a waste barrel (standard 55 gallon drum) attached to the SCB.

Depending on the degree of waste compaction, up to 14 targets and associated waste may fit in a single barrel; however, the ^{235}U content of each barrel is limited to 350 g. by DOT regulations. As each barrel is filled, the ^{235}U inventory will be monitored, and additional fissile material will not be added to the barrel once the fissile limit is reached (e.g. only 11 targets, if each contained 30 g. ^{235}U , could be loaded into a barrel to remain below the 350 g. limit). When a barrel is full, either volumetrically or having reached a total ^{235}U inventory of 350 g., it will be moved temporarily into the elevator pit, which can hold up to 5 barrels. At some convenient time after 4 barrels are accumulated, the barrels will be loaded on a waste cart which will then be moved into Room 109. Up to 25 carts, some containing 8 and some containing 4 waste barrels, with a total of 180 barrels, can be accommodated in Room 109.

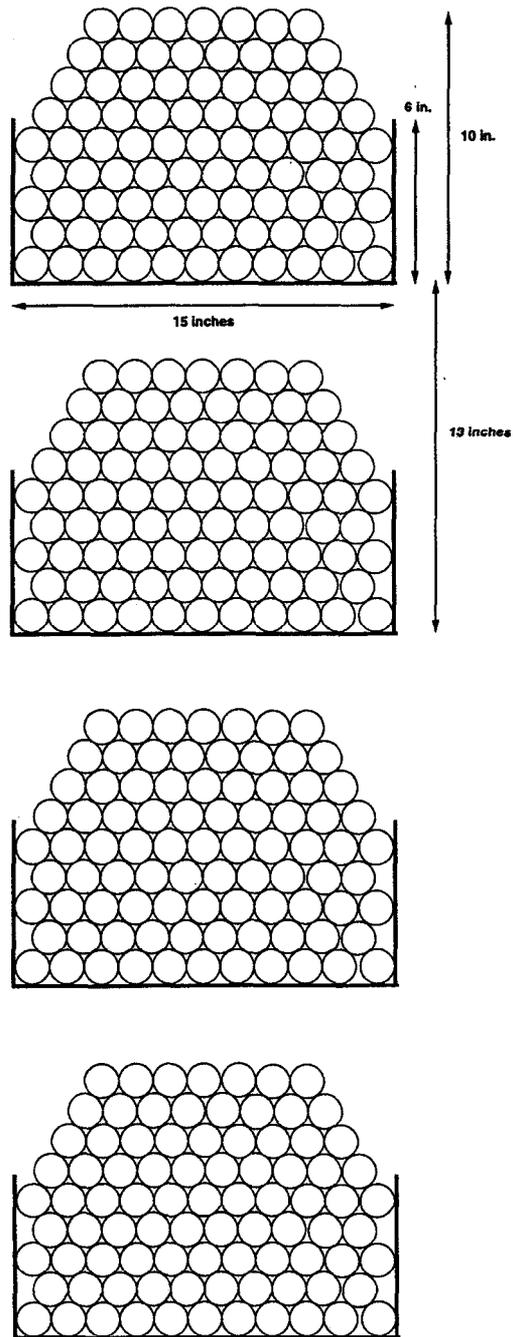


Figure 6. MCNP Model of Storage Drawer with 88 Cintichem Targets.

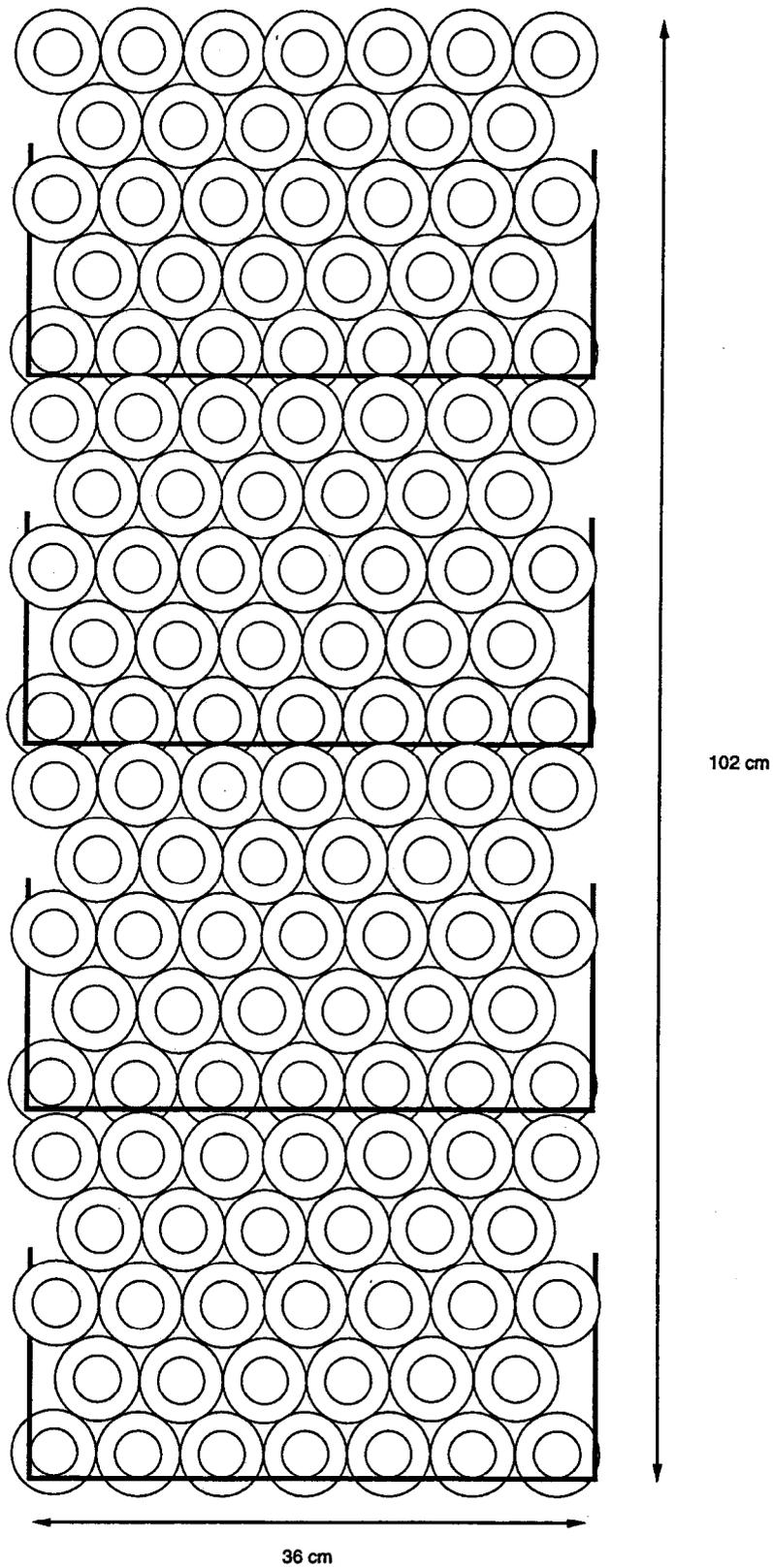


Figure 7. Array of 156 targets at a 4.5 cm pitch.

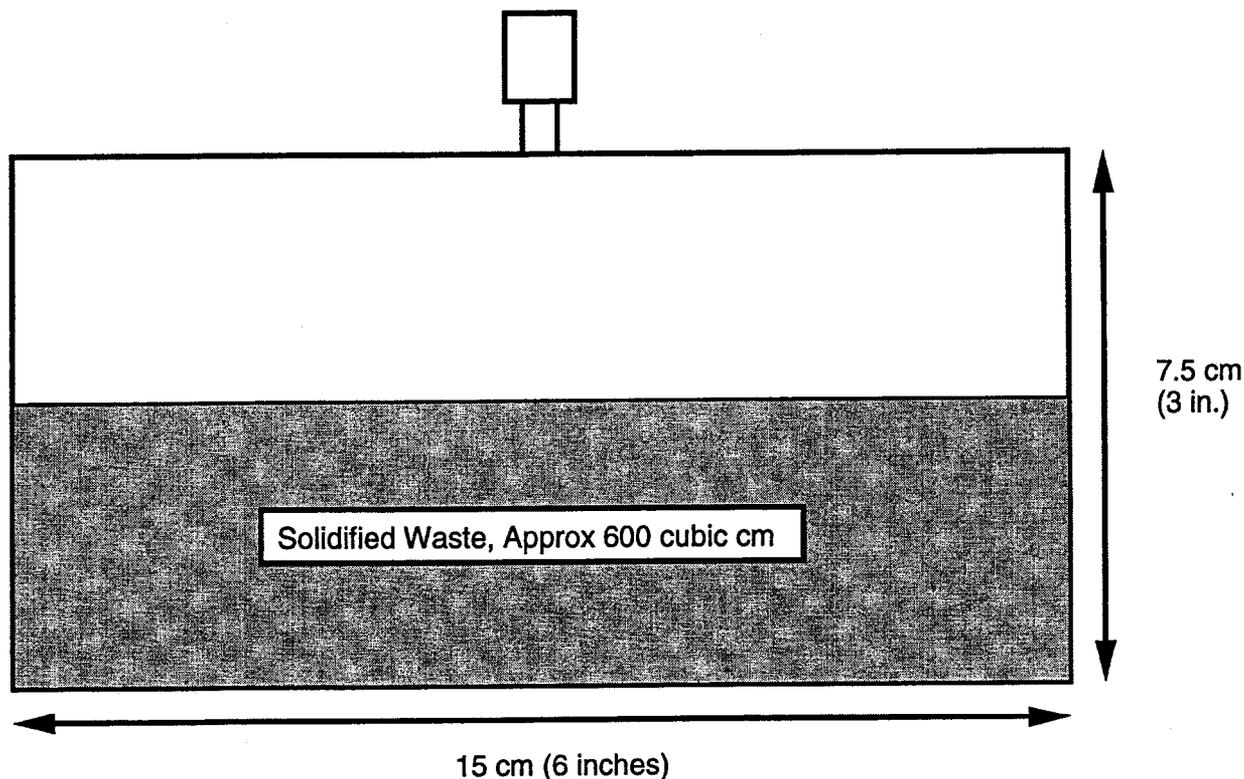


Figure 8. Waste container with solidified concrete waste.

The waste storage configuration was modeled in four different ways to evaluate configurations which have the potential to produce the greatest neutron multiplication. These hypothetical configurations are not necessarily physically achievable. The analyses were accomplished parametrically to support the conclusion that the most reactive configurations were evaluated.

In each barrel, the proximity and atom densities of fissile materials and moderator are limited by the solid concrete waste and the waste containers, as depicted in Figure 9. The waste associated with 14 targets will be contained in 8.4 liters of concrete, containing about 4 liters of water, and held in stainless steel containers which occupy a volume of about 18 liters in the barrel. Normally, these containers would be dispersed in the barrel, but analyses of configurations which evaluated both the agglomeration of the materials as well as the dispersal of the materials, were accomplished to provide perspective for the parameters important for criticality consideration. Thus the analyzed configurations represent a considerable range of fissile material as well as moderator densities, well beyond what could credibly be achieved in either normal or accident conditions. The analyses were performed over a considerable span of time by different individuals, so the details and configurations used in the analyses vary. However, the results and conclusions of the analyses are valid and applicable to the waste storage scenario.

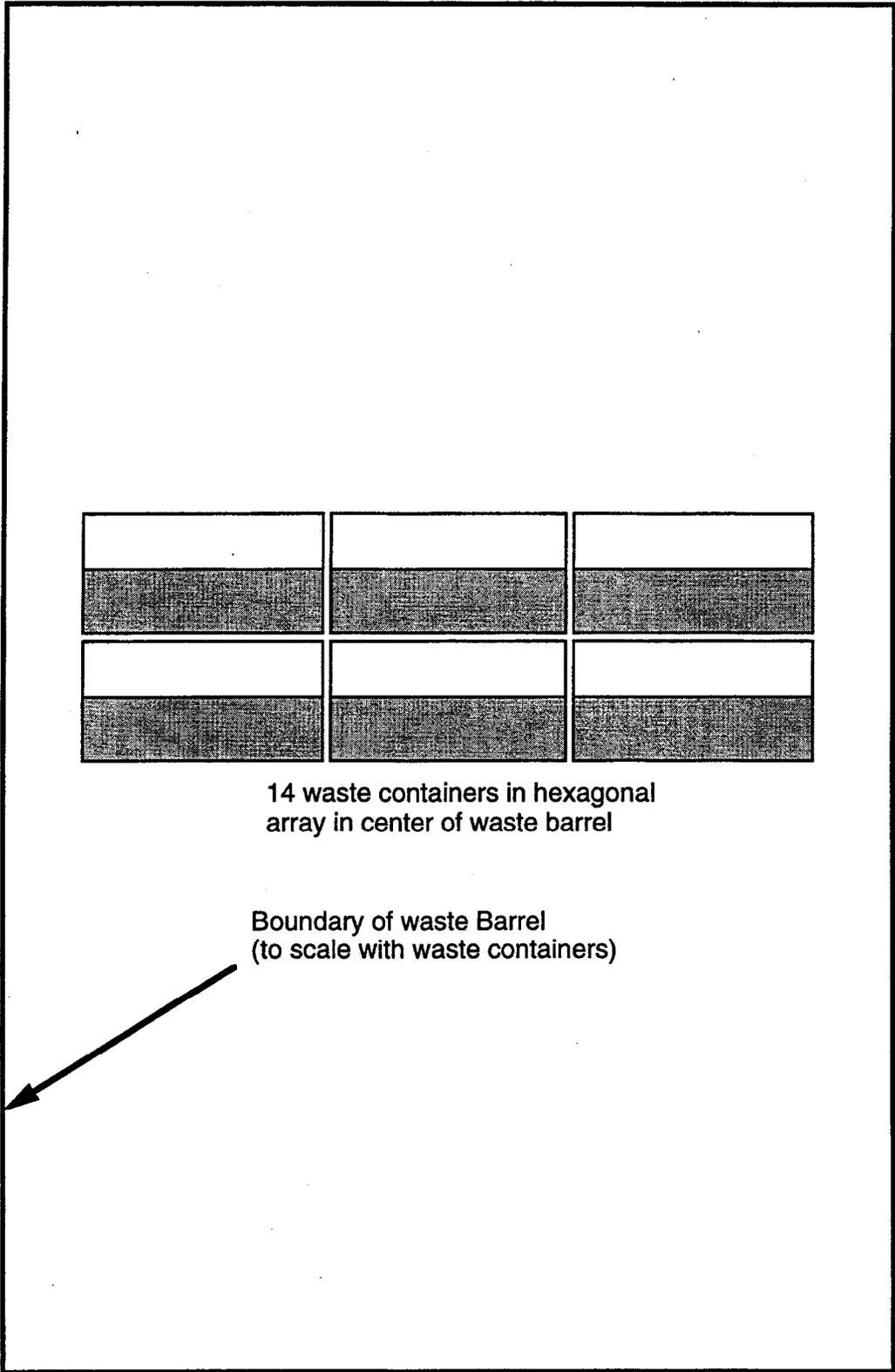


Figure 9. Close packed waste containers in a waste Barrel.

The first configuration analyzed assumed that all of the ^{235}U in the barrel was assimilated into a single sphere, with a total volume of 4 liters. This is based only on the volume of water in the concrete, representing the solidified waste resulting from 14 targets (i.e. neglecting the fact that the steel waste containers would preclude an assimilation to a volume of less than about 18 liters). It is also assumed that the process solution combined with the concrete is represented by water, which remains in the concrete mixture. Thus, the waste in each barrel is represented by a 4-liter sphere consisting of ^{235}U in a water solution, centered in the barrel, as shown in Figure 10. The overall configuration of barrels in Room 109 is shown in Figure 3. This analysis configuration will be identified as WS1. The presence of the stainless steel waste canister, stainless steel targets, stainless steel waste barrel, and other process materials in each barrel were neglected, which should conservatively bias the results due to neutron absorption which would occur if these materials were represented. Two mass loadings of fissile ^{235}U were evaluated for this geometry: 423 g. ^{235}U (1.8 moles), representing 14 targets each containing 30 g ^{235}U ; and 350 g. ^{235}U (1.5 moles), representing a barrel conforming to DOT regulations. For both mass loadings, the mass of water was kept constant at 3960 grams H_2O (220 moles), yielding H/U ratios for these configurations of 290 and 245. The fissile/water spheres are arranged in a $9 \times 10 \times 2$ square pitch or lattice array, based on the dimensions of a waste barrel (56-cm diameter and 86 cm high). Such an array would contain 180 spheres containing a total of 63 to 76 kg of ^{235}U . The entire array was reflected with a 10-cm water reflector. Configurations with and without water occupying the space between the 4-liter spheres were analyzed.

A second evaluation of the waste storage configuration was evaluated by assuming that 350 g. of ^{235}U is suspended in water solution in a right circular cylinder centered in the waste barrel. The amount of water in the cylinder is varied from 58 grams (H/U=4) to 236 kg (H/U= 17,600), representing an entire waste barrel full of water/ ^{235}U solution. It should be noted that while these analyses in most cases represent physically unrealizable geometries, they span the range of potential neutron multiplication. The geometry of this configuration is illustrated in Figure 11, while the overall barrel storage configuration remains as depicted in Figure 3. These analyses were accomplished for an array of 160 barrels instead of 180 barrels, and this analysis configuration is identified as WS2. Water reflection around each barrel was also evaluated, although the effects of such reflection are not large (5% to 10%) for configurations which are near optimally moderated, as would be expected. The steel waste barrel was modeled as 18 gauge (.13 cm), whereas actual drums are 16 gauge (.15 cm). However, the steel waste containers, steel targets, and other waste materials were neglected for the purposes of the calculation. These assumptions should yield conservative results, since the additional steel will reduce effective multiplication.

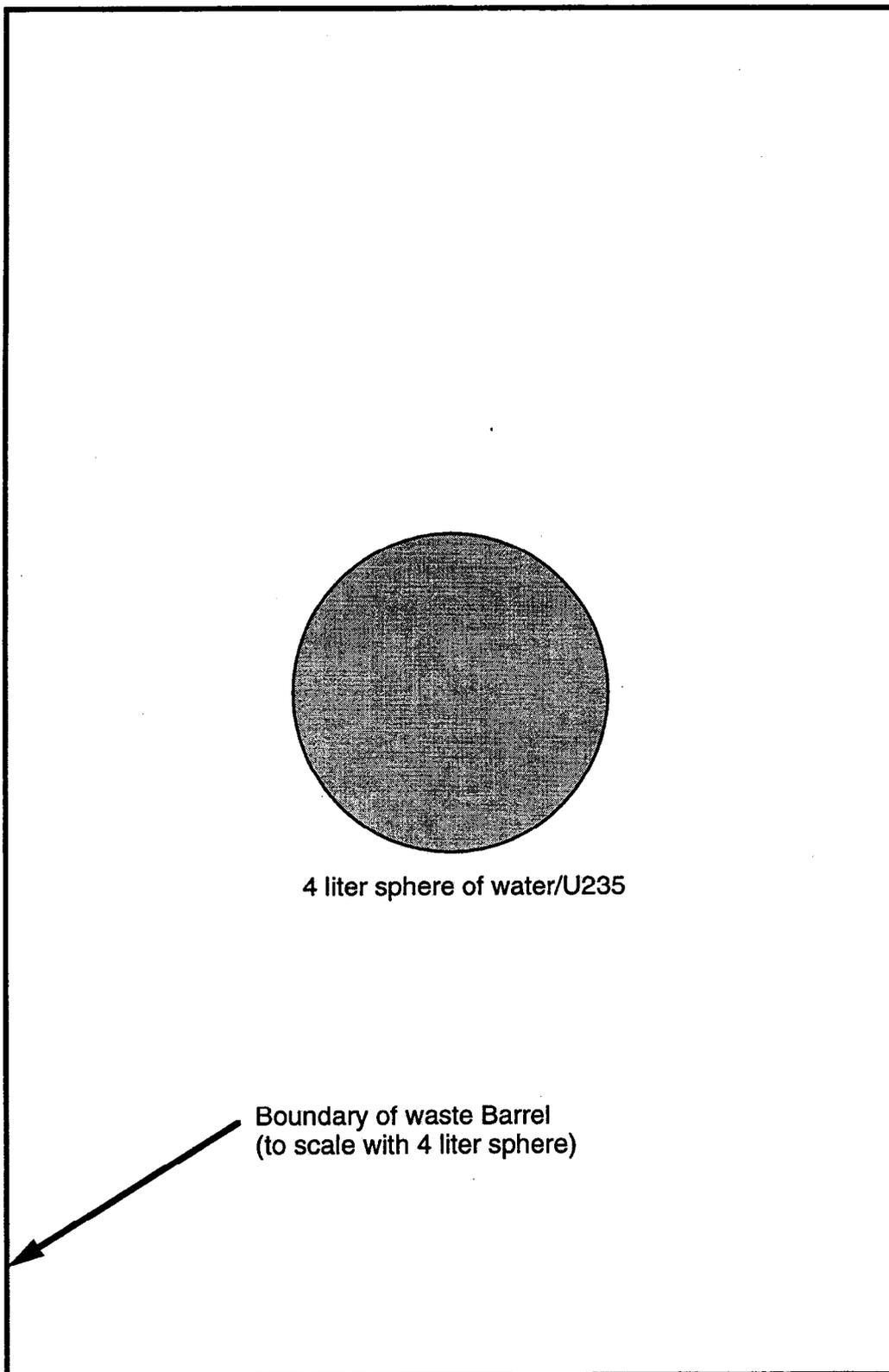


Figure 10. Spherical waste configuration in a barrel (WS1).

Figures 11 & 12. Cylindrical & Hemispherical Geometries.

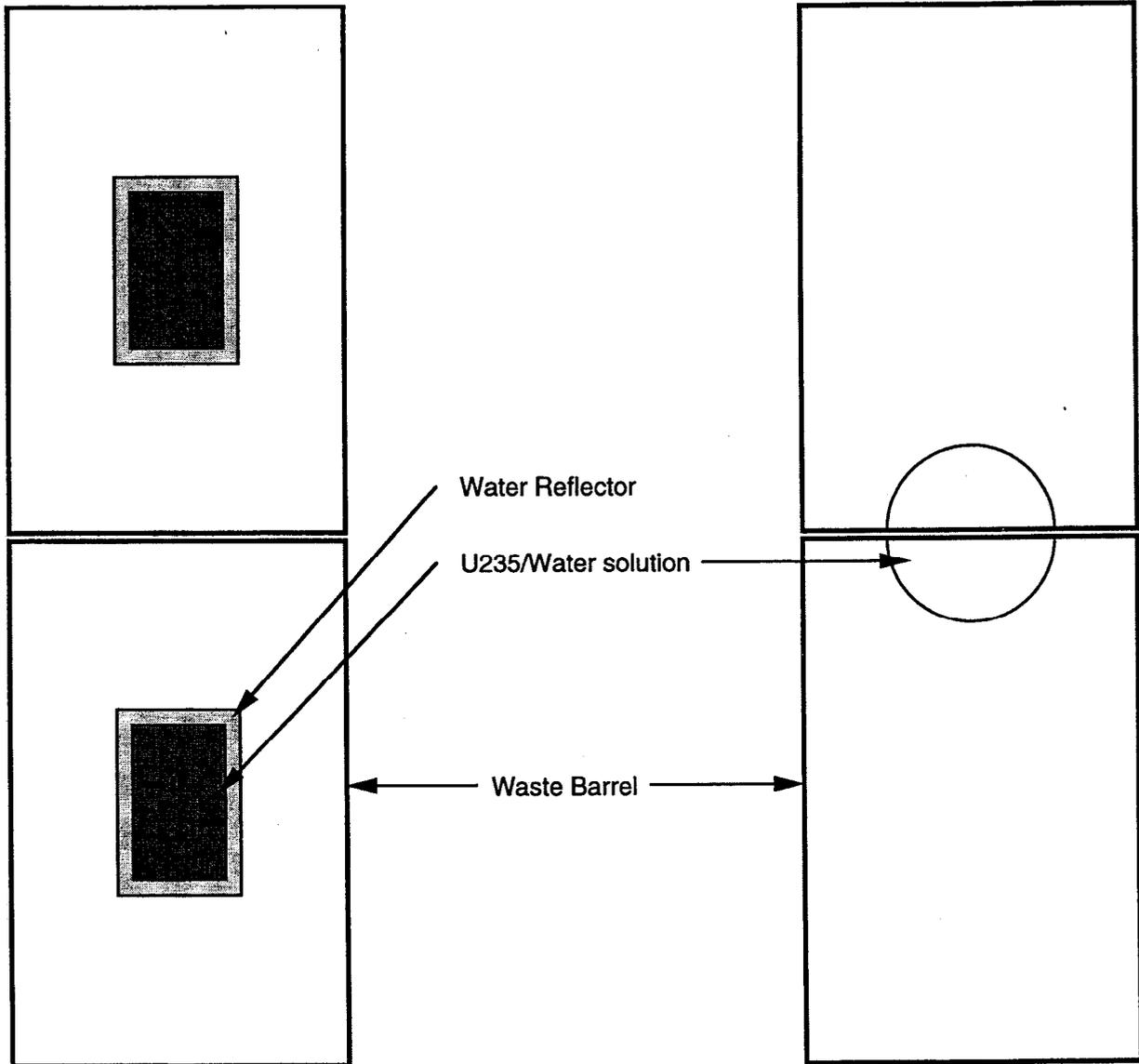


Figure 11. Waste in Barrel, Cylindrical Geometry (WS2).

Figure 12. Waste in Barrel, Hemispherical Geometry (WS3).

Thirdly, the waste was modeled as opposing hemispheres in each vertical pair of waste barrels, with the H/U ratio parametrically varied from 132 to 2040, both with and without reflection by water. The separation of the hemisphere face is constrained by the barrel storage geometry to be no closer than 2.28 cm (0.9 in.). This geometry is illustrated in Figure 12, and is identified as configuration WS3.

Finally, to assess the degree to which the above-analyzed configurations represent maximum neutron multiplication, an array was evaluated as barrels in which the ^{235}U was uniformly dispersed and the water (hydrogen) atom density was varied over a wide range. This configuration is essentially identical to the full waste barrel described as configuration WS2, except that the water atom density is reduced. The array was modeled as an infinite planar array of barrels stacked two high rather than a configuration of 160 or 180 barrels.

6.3 Results of Analyses

6.3.1 Target Storage Results

A sample copy of an MCNP input and output file for the target storage configuration is included in Appendix A. Table 1 presents the k_{eff} results for the target storage scenario. Results are presented for a dry array of targets at a pitch of 3.2 cm. where: the interstitial space between the targets is flooded with water; the safe is reflected by 10 cm of water; and where in addition to water between the targets, 10%, 20%, 50%, and 100% of the targets are also internally filled with water (Romero, 1998d). The statistical uncertainty of the results ranges from 0.002 to 0.0026, but is not shown in the table for ease of depiction.

Table 1. Results for Storage of Cintichem Targets in a Safe.

Targets per Drawer	Base Case (dry)	Externally Flooded & Reflected	10% Internally Flooded	20% Internally Flooded	50% Internally Flooded	100% Internally Flooded
88	0.0156	0.520	0.583	0.641	0.825	1.03
79	0.0145	0.485	0.544	0.613	0.782	0.991
69	0.0134	0.458	0.513	0.576	0.737	0.942
39	<0.01	0.831	0.857	---	---	0.972

The results for 39 targets in each drawer, at a pitch of 4.5 cm and a drawer spacing of 25.4 cm, is shown in the last row of Table 1 (Romero, 1998a). For this geometry where the array is externally flooded, the effective multiplication increases significantly as compared to the close packed configurations, from about 0.5 to 0.83, due to the effects of water moderation. The magnitude of these effects change as the degree of internal flooding of the targets increases, as indicated by the variation of less than 10% in neutron multiplication over a range of 39 to 88 targets per drawer. With all targets internally filled with water, a pitch of 3.2 cm is near optimum for neutron multiplication (Romero, 1998a).

Significant internal flooding of targets in storage configurations is assessed to be incredible based on the following:

1. The integrity of each target and its cap, using helium mass spectrometer techniques, is ascertained as part of the receiving inspection. This inspection is rigorously observed for production quality assurance and for ACRR irradiation safety requirements. The likelihood of a target failing this inspection and stored for future use is low, but subject to human error, is a possible event. The assessed probability is probably less than 1%, however; observation of improperly sealed targets at a rate much above 0.1% would likely lead to a management review for procedure adequacy.

2. If the target cap is not securely tightened, significant quantities of water will not readily enter the target due to the surface tension of water which would bridge small gaps in a loosely fitted cap. However, even if the effect of surface tension is ignored, with an individual probability of an unsealed target of 1%, the likelihood of more than 6% of a group of targets having unsealed caps is calculated to be less than 1E-6, based on the binomial distribution:

$$P(x) = n! p^x (1-p)^{n-x} / (x!(n-x)!) \quad x = 0, 1, 2, 3, \dots n$$

where: $P(x)$ is the probability of exactly x events
 n is the number of trials
 p is the probability of an event

Thus, the maximum effective multiplication factor for storage of up to 352 targets, each containing 30 g. of ^{235}U in a safe (even if externally flooded, including the maximum bias of 0.005 and the statistical uncertainty of .0026) is calculated based on the results summarized in Table 1 to be highly subcritical, with a k_{eff} of less than 0.6 (three sigma). Based on these results, criticality in storage configurations in a safe is not considered credible.

6.3.2 Waste Storage Results

Results for the waste storage configurations represented by 180 spheres of uranium in water solution, are presented in Table 2 for 4-liter spheres containing 350 g. and 423 g. of ^{235}U (Configuration WS1). All WS1 configurations, with and without flooding, are calculated to remain subcritical, with the maximum calculated multiplication, including bias and statistical uncertainty, of 0.8 for configurations containing 350 g. per barrel (Romero, 1998e).

**Table 2. Results for 180 4.0L Spheres.
(Homogenous mixture of ^{235}U and H_2O)**

^{235}U loading (grams)	Bare spheres, no reflector ($k_{\text{eff}} \pm \sigma$)	Reflected array ($k_{\text{eff}} \pm \sigma$)	Flooded and reflected array ($k_{\text{eff}} \pm \sigma$)
423	0.580 ± 0.0026	0.695 ± 0.0031	0.820 ± 0.0027
350	0.554 ± 0.0027	0.663 ± 0.0027	0.791 ± 0.0028

These MCNP results are quite consistent with the separately modeled KENO results (WS2 and WS3 configurations) shown in Figure 13 for both cylindrical and spherical configurations of arrays of 160 barrels of waste each containing 350 g ^{235}U (Vernon, 1998). The WS1 configuration k_{eff} result for a flooded and reflected array of 0.79 compares with a calculated k_{eff} of 0.75 for a reflected WS2 cylindrical array at an H/U of 300, which is the moderator ratio for the WS1 configuration. Given the difference in geometry, degree of reflection/moderation, and analytical methods for these two separate analysis, these are quite consistent results. These analyses (Romero, 1998e) also indicate that the effective multiplication of 160 barrel arrays and 180 barrel arrays are not significantly different.

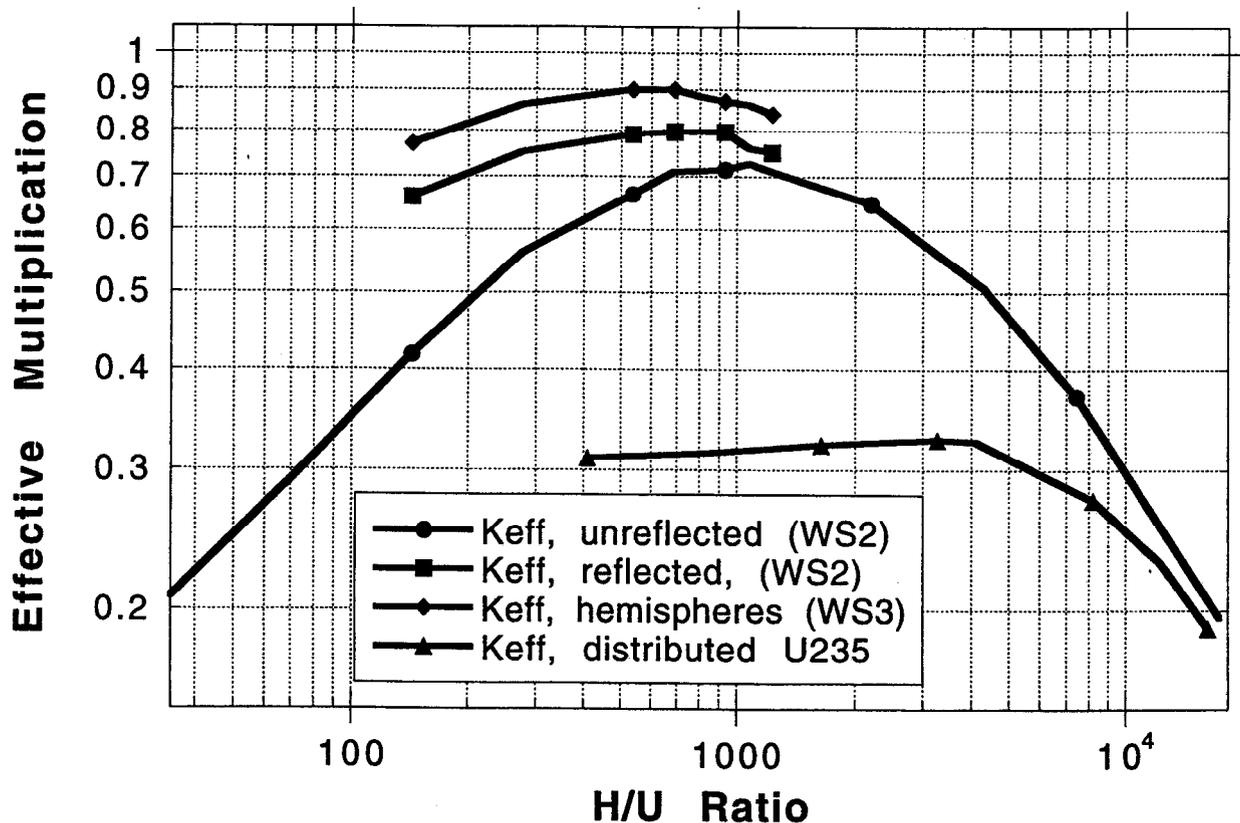


Figure 13. Criticality Analyses Results.

As depicted in Figure 13, a maximum k_{eff} of 0.72 is calculated for the unreflected WS2 cylindrical configuration, 0.8 for the reflected WS2 cylindrical configuration, and 0.9 for the hemispherical WS3 configuration. Maximum neutron multiplication for these configurations occurs at an H/U ratio of between 600 and about 1000, which equates to 8 to 14 kg (liters) of water; as compared to the 4 kg used for the MCNP (WS1) analysis, which represents a more realistic configuration. In fact, once the waste is solidified in concrete, additional water assimilation into the waste is effectively precluded, even in flooded configurations. At an H/U of 300, which represents the maximum quantity of water which would realistically be present in the concrete, the k_{eff} for the centered cylindrical geometry (WS2) is calculated to be about 0.75, while for the hemispherical geometry it is about 0.86. The WS2 and WS3 results for reflected cases are plotted at the maximum effective multiplication value (optimum reflection) which is parametrically calculated. Thus, the analytical results are plotted conservatively. The amount of water reflector varies in each case from a few cm up to about 10 cm around each barrel.

The analyses of the configuration in which the ^{235}U is uniformly distributed in the barrel and the water density is varied is also plotted in Figure 13, with a peak multiplication of about 0.32, to illustrate the degree to which the analyses described in this assessment evaluates configurations with maximum neutron multiplication (Romero, 1999).

Both the MCNP and the KENO analyses indicate that criticality in waste storage configurations (both in Room 109 and in the elevator pit, where only 5 barrels of waste will be stored) of maximally loaded barrels remain subcritical in normal, abnormal, and even in accident and incredible scenarios involving water flooding and geometrical redistribution of ^{235}U . Maximum

effective multiplication, even for highly moderated and reflected geometries which are physically unrealizable due to the form and storage configuration of the waste, are expected to remain subcritical by a significant margin as shown in Figure 13. Additionally, the calculations in Table 2 indicate that for the configuration where the ^{235}U remains in the concrete, the results are not highly sensitive to ^{235}U loading, as indicated by only a 3% increase in effective multiplication with a 20% increase in fissile content. Thus, in addition to flooding and geometrical redistribution, significant and multiple oversights of target fabrication, target inspection, process chemistry, and/or fissile material tracking would be required to result in a criticality accident. Based on the above results, accidents and/or oversights which would result in criticality in a waste storage configuration are not considered credible in the HCF.

7.0 Design Features (Passive and Active) and Administratively Controlled Limits and Requirements

A large number of design features and administrative limits will effectively preclude the possibility of a criticality accident in the HCF. Many of these features and limits exist for reasons other than criticality, but will be described to provide a sense of the defense in depth which exists to preclude accidental criticality. Those features and limits, which are specifically relied on to preclude criticality, will be separately and specifically identified.

7.1 General Discussion of Design Features and Limits

Processing of isotope targets containing ^{235}U is rigorously governed by procedure. Process throughput will require that material flow through the HCF not be restricted and allowed to accumulate at any point, or it will constrain follow-on production. Thus, the possibility of inadvertent accumulation of fissile materials is highly unlikely in that such accumulation would prevent additional production. Furthermore, such accumulation would be readily apparent and will be monitored on a near continuous basis during production operations.

Maximum processing rates of 6 targets per day restrict the quantity of material at risk of criticality at any one time. Multiple, independent errors in process control would be required to permit accumulations which would result in a critical configuration. Furthermore, errors would need to occur repeatedly over multiple days, and would have to go unnoticed in a rigorous production environment.

Both engineered features and administrative limits will preclude inadvertent criticality in the HCF. Engineered features include:

- Target design, which constrains the amount of ^{235}U in a single target.
- Target sealing features which preclude internal flooding.
- Target volume which limits packing density.
- Fuel form as UO_2 .
- Volume of process containers & quantities of liquid (moderating) materials.
- Physical space available for target processing which constrains collocation.
- Physical isolation of process boxes.
- Waste form as concrete.
- Waste container design.

- Physical volume required for residual materials which limits accumulation quantity.
- Storage array design which controls storage geometry.

These features physically preclude the accumulation of significant quantities of ^{235}U in process boxes within Zone 2A. Normally, ^{235}U in any single process box would be limited by these features to less than 60 g. ^{235}U (two targets). Unusual circumstances might cause up to 6 targets to be present in a box, which would total less than 200 g. ^{235}U . In these situations, the likely configuration of the majority of the targets would be as unprocessed but sealed targets, which would preclude the intermixing of water or moderating materials with the fissile material.

Accumulation of waste containing fissile ^{235}U is limited by volumetric considerations to about 420 g. ^{235}U per waste barrel, and DOT regulations require less than 350 g. per barrel, which will be administratively controlled in the HCF. Physical space constraints in Zone 2A will limit the number of waste barrels to five or less, or up to 1.75 kg ^{235}U . The concrete waste form at this time and physical spacing due to the containerization will preclude a critical configuration, even in abnormal and accident configurations. In the waste storage room, the volume of the room and the volume of the barrels physically limits the quantity of fissile material that can be emplaced and also establishes sufficient spacing between fissile containers.

Administrative controls supplement engineered features to preclude an inadvertent criticality. These controls include:

- Limitation of the number of targets or target residuals within a process box.
- Limitation of the number of targets which may be stored in a safe or cabinet.
- Limitations on the number of targets which can be in-process (liquid) at any one time.
- Limitations on the quantity of liquids which will be introduced into the process boxes.
- Limitations on the quantity of ^{235}U contained in a single storage barrel.
- Limitations on the total quantity of ^{235}U that can be stored in Room 109.

These limitations are embodied in HCF operating procedures and/or production procedures, reviewed by cognizant safety committees, and approved by HCF line management.

7.2 Design Features and Administrative Limits Required to Prevent Criticality

The analyses presented in this CSA assume a maximum target fissile loading of 30 g. of ^{235}U . Routine processing of targets loaded to greater than 30 g. will require additional analyses. Additionally, the dimensions and material of the target tube form the basis for storage analyses. These aspects of the design should not be changed without an evaluation of the effects on storage criticality limitations. Target inspections and verifications provide assurance that the target characteristics conform to the design. These inspections and verifications should not be compromised without assessing the potential impacts on criticality.

For target storage configurations, 352 unirradiated targets per safe, with a total safe content of 10.5 kg ^{235}U would be subcritical under all credible conditions based on the analyses described in this CSA. However, each safe will be administratively limited to no more than 6 kg to alleviate security requirements based on SNM Category. Target storage safes shall be separated by a distance of no less than 6 feet to preclude neutronic coupling.

In the case of the process boxes within Zone 2A, and for any other unanalyzed storage locations, ^{235}U mass is administratively limited to less than 350 g. per location. This mass is one half of the safe mass of 700 g. of ^{235}U in aqueous solution established in GN470072. This limit precludes criticality even in flooding scenarios.

For waste storage in Room 109, administrative limits are used to limit the quantity of ^{235}U in each waste barrel to no more than 350 g. A room total fissile limit of 50 kg will be established to maintain quantities of SNM below DOE M 474.1-1A specifications for Category III D, which is the appropriate categorization for the material in the waste form, since the waste contains less than 10 weight percent ^{235}U . These quantities of ^{235}U have been analyzed as described in this CSA to remain subcritical in any credible configuration, however some reliance on spacing provided by the waste barrels is inherent in the analyses. Thus, storage in prescribed waste barrels should be observed. An inventory of all waste emplaced in Room 109 will be maintained for waste disposal and SNM purposes.

In summary, the design features and administrative limits that are relied upon to prevent criticality in the HCF are:

- Target ^{235}U content is limited to 30 g. and target integrity is verified by physical inspection or by fabrication or receipt records that document the fissile loading; diameter and length dimensions, seal integrity, and material form, i.e. UO_2 . [Note: Records inspection should be sufficient unless there is obvious physical damage to a target.]
- Changes to the design of the target tube require criticality review.
- Up to 352 targets (88 per drawer), but no more than 6-kg ^{235}U can be stored in any safe.
- For multiple safe configurations containing greater than 350 grams ^{235}U (total), spacing between safes shall be 6 feet or greater.
- SCB's in the HCF are singularly and collectively limited to a maximum of six targets.
- No more than 350 grams ^{235}U can be placed in each waste barrel.
- Waste barrels shall be standard 55-gallon drums.
- No more than 50 kg ^{235}U can be stored in Room 109.
- For multiple safes, surface spacing between safes shall be 6 feet or greater.

These features and limits will be implemented either in the form of HCF administrative procedures, TSR's, or Medical Isotope Program design control procedures.

8.0 Summary and Conclusions

A number of fissile material storage configurations representing unirradiated target storage and waste material storage have been evaluated in this CSA. These evaluations indicate that the planned storage configurations remain subcritical under all credible circumstances. Both design features and administrative controls provide assurance that criticality is not a credible event, and the features and controls that preclude criticality are specifically identified. Double contingency has been evaluated in this CSA and the planned HCF operations adhere to the double contingency principle.

References

- Bodette, David, (1996), "Benchmarking MCNP Calculations," Memorandum to File, Sandia National Laboratories, Albuquerque, NM, July 11, 1996.
- Briesmeister, Judith F. (ed.), (1993), *MCNP - A General Monte Carlo N-Particle Transport Code, Version 4A*, LA-12625-M Manual, Rev. 2, Los Alamos National Laboratory, Los Alamos, NM, November 1993.
- DOE Order 5480.21, (1991), "Unreviewed Safety Questions", U.S. Department of Energy, Washington, DC, December 24, 1991.
- DOE Order 5480.23, (1992), "Nuclear Safety Analysis Report", U.S. Department of Energy, Washington, DC, April 10, 1992.
- DOE STD-3007-93, (Change Notice No. 1, September 1998), (1993), "Guidelines for Preparing Criticality Safety Evaluations at Department of Energy Non-Reactor Nuclear Facilities", U.S. Department of Energy, Washington, DC, November 1993.
- DOE O 420.1 (Chg. 2: October 24, 1996), (1995), "Facility Safety", U.S. Department of Energy, Washington, DC, October 13, 1995.
- DOE M 474.1-1A, (2000), "Manual for Control and Accountability of Nuclear Materials", U.S. Department of Energy, Washington, DC, November 22, 2000.
- Miles, Robert E., (1985), "KENO 5A-PC Monte Carlo Criticality Program with Supergrouping," Instruction Manual CCC-548, April 1985.
- Miller, Dennis L., (1996) "Target Coating Information," Memorandum to Cecil Tucker, Sandia National Laboratories, Albuquerque, NM, Feb. 19, 1996.
- Mitchell, Gerry W., Naegeli, Robert E., Mahn, Jeffrey A., Longley, Susan J., Philbin, Jeffrey S., Schwers, Norman F., Vanderbeek, Thomas E., and Berry, Donald T., (2000), *Hot Cell Facility (HCF) Safety Analysis Report*, SAND2000-2355, Sandia National Laboratories, Albuquerque, NM, November 2000.
- Parma, Edward J., (1997), "Criticality calculations for Cintichem Targets," Memorandum to J. W. Bryson and F. M. McCrory, Sandia National Laboratories, Albuquerque, NM, Sept. 23, 1997.
- Philbin, Jeffrey S., (1998), Supplement GN470072 to the SNL ES&H Manual, "Nuclear Criticality Safety", Sandia National Laboratories, Albuquerque, NM January 28, 1998.
- Romero, Daniel, (1998a), "Criticality safety assessment for storage of medical isotope targets and process waste," Memorandum to G. W. Mitchell, Sandia National Laboratories, Albuquerque, NM, April 10, 1998.

Romero, Daniel, (1998b), "Comparison of MCNP and KENO Parametric Studies for Hot Cell Process Waste Storage," Memorandum to G. W. Mitchell, Sandia National Laboratories, Albuquerque, NM, October 2, 1998.

Romero, Daniel, (1998c), "Parametric study of keff vs. water density for various target pitches," Memorandum to Distribution, Sandia National Laboratories, Albuquerque, NM, June 30, 1998.

Romero, Daniel, (1998d), "Parametric study of keff for the Storage of Cintichem-type targets," Memorandum to G. W. Mitchell, Sandia National Laboratories, Albuquerque, NM, October 1, 1998.

Romero, Daniel, (1998e), "Hot Cell Process Waste Storage Parametric Studies," Memorandum to G. W. Mitchell, Sandia National Laboratories, Albuquerque, NM, October 7, 1998.

Romero, Daniel, (1999), "Evaluation of k_{∞} for Hot Cell Facility Process Waste Storage," Memorandum to G. W. Mitchell, Sandia National Laboratories, Albuquerque, NM, January 5, 1999.

Vernon, Milton. E., (1998), "Criticality Analyses," Memorandum to R. L. Coats, Sandia National Laboratories, Albuquerque, NM, May 26, 1998.

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```

1200 py 115.57
c
c water reflector surfaces
110 px 29.06 $right reflector surface
120 px -29.06 $left reflector surface
130 py 125.57 $top reflector surface
140 py -26.51 $bottom reflector surface
150 pz 32.86 $back reflector surface
160 pz -32.86 $front reflector surface

```

```

c
c MATERIAL CARDS
c
kcode 1000 1.0 10 110
ksrc 1.52 -1.15 0 0 0.37 0
      -1.52 -1.15 0 0 -2.67 0

```

```

c
c UO2 layer in target
c 30.0 g U235
m1 92235.50c 0.02743 $uranium-235
    92238.50c 0.00204 $uranium-238
    8016.50c 0.05893 $oxygen
c
c water moderator (1.0 g/cc)
m2 1001.50c 2.00 $hydrogen
    8016.50c 1.00 $oxygen
mt2 lwtr.01t $water T=300 K
c
c SS304 target clad (7.92 g/cc)
m3 26000.50c -0.695 $iron
    24000.50c -0.190 $chromium
    28000.50c -0.095 $nickel
    25055.50c -0.020 $manganese-55
prdmp 50 50 0 1

```

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=====
estimator cycle 110 ave of 100 cycles combination simple average combined average corr
k(collission) 0.617731 0.639959 0.0033 k(col/abs) 0.640426 0.0033 0.640102 0.0034 0.9746
k(absorption) 0.626775 0.640893 0.0034 k(abs/tk ln) 0.642224 0.0036 0.641325 0.0033 0.4876
k(trk length) 0.676702 0.643555 0.0049 k(tk ln/col) 0.641757 0.0036 0.640461 0.0033 0.5057
rem life(col) 1.1909E+04 1.0884E+04 0.0039 k(col/abs/tk ln) 0.641469 0.0033 0.640621 0.0034
rem life(abs) 1.1925E+04 1.0883E+04 0.0040 life(col/abs) 1.0884E+04 0.0040 1.0884E+04 0.0040
0.9984
source points generated 1016

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1problem summary

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run terminated when 110 kcode cycles were done.

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+ target storage safe criticality calculation 09/29/98 21:19:41
0 probid = 09/29/98 20:06:16

```

neutron creation	tracks	weight	energy	neutron loss	tracks	weight	energy
	(per source particle)			(per source particle)			
source	109613	1.0035E+00	2.0431E+00	escape	20662	1.3983E-01	1.3543E-01
weight window	0	0.	0.	energy cutoff	0	0.	0.
cell importance	0	0.	0.	time cutoff	0	0.	0.
weight cutoff	0	9.4851E-02	1.1578E-07	weight window	0	0.	0.
energy importance	0	0.	0.	cell importance	0	0.	0.
dxtran	0	0.	0.	weight cutoff	88956	9.5541E-02	1.1167E-07
forced collisions	0	0.	0.	energy importance	0	0.	0.
exp. transform	0	0.	0.	dxtran	0	0.	0.
upscattering	0	0.	5.6901E-07	forced collisions	0	0.	0.
				exp. transform	0	0.	0.
(n,xn)	10	7.9100E-05	5.2727E-05	downscattering	0	0.	1.8802E+00
fission	0	0.	0.	capture	0	5.9930E-01	1.9935E-02
total	109623	1.0985E+00	2.0432E+00	loss to (n,xn)	5	3.9550E-05	3.8205E-04
				loss to fission	0	2.6374E-01	7.2478E-03
				total	109623	1.0985E+00	2.0432E+00

number of neutrons banked	5	average lifetime, shakes		cutoffs
neutron tracks per source particle	1.0001E+00	escape	5.8820E+03	tco 1.0000E+34
neutron collisions per source particle	1.7237E+02	capture	1.1678E+04	eco 0.0000E+00
total neutron collisions	18893506	capture or escape	1.0870E+04	wc1 -5.0000E-01
net multiplication	1.0000E+00 0.0002	any termination	1.2740E+04	wc2 -2.5000E-01
computer time so far in this run	73.42 minutes	maximum number ever in bank	1	
computer time in mcrun	72.04 minutes	bank overflows to backup file	0	
source particles per minute	1.5216E+03	field length	0	
random numbers generated	152583972	most random numbers used was	10678 in history	20466

keff estimator	keff	standard deviation	68% confidence	95% confidence	99% confidence
collision	0.63996	0.00212	0.63784 to 0.64208	0.63575 to 0.64417	0.63437 to 0.645
absorption	0.64089	0.00215	0.63874 to 0.64305	0.63660 to 0.64518	0.63520 to 0.646
track length	0.64355	0.00317	0.64038 to 0.64673	0.63724 to 0.64987	0.63517 to 0.651
col/absorp	0.64010	0.00216	0.63794 to 0.64227	0.63579 to 0.64441	0.63438 to 0.645
abs/trk len	0.64133	0.00212	0.63920 to 0.64345	0.63710 to 0.64556	0.63571 to 0.646
col/trk len	0.64046	0.00211	0.63835 to 0.64257	0.63626 to 0.64466	0.63489 to 0.646
col/abs/trk len	0.64062	0.00216	0.63846 to 0.64278	0.63632 to 0.64492	0.63492 to 0.646

if the largest of each keff occurred on the next cycle, the keff results and 68, 95, and 99 percent confidence interval

keff estimator	keff	standard deviation	68% confidence	95% confidence	99% confidence
collision	0.64042	0.00215	0.63828 to 0.64257	0.63615 to 0.64470	0.63476 to 0.646
absorption	0.64131	0.00217	0.63914 to 0.64349	0.63698 to 0.64564	0.63557 to 0.647
track length	0.64415	0.00320	0.64095 to 0.64735	0.63778 to 0.65051	0.63570 to 0.652
col/abs/trk len	0.64115	0.00219	0.63896 to 0.64334	0.63679 to 0.64551	0.63537 to 0.646

the estimated collision/absorption neutron lifetimes, one standard deviations, and 68, 95, and 99 percent confidence in

type	lifetime(sec)	standard deviation	68% confidence	95% confidence	99% con
removal	1.0884E-04	4.3177E-07	1.0841E-04 to 1.0927E-04	1.0798E-04 to 1.0970E-04	1.0770E-04 t
capture	1.1697E-04	3.8099E-07	1.1659E-04 to 1.1735E-04	1.1621E-04 to 1.1773E-04	1.1597E-04 t
fission	8.5250E-05	3.8034E-07	8.4869E-05 to 8.5630E-05	8.4492E-05 to 8.6007E-05	8.4245E-05 t
escape	5.8972E-05	6.8983E-07	5.8281E-05 to 5.9662E-05	5.7597E-05 to 6.0346E-05	5.7149E-05 t

1 average individual and combined collision/absorption/track-length keff results for 7 different batch sizes

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Appendix B

Sample I/O for Processed Target Waste Storage Array

Storage Configuration WS1

The following is a sample MCNP input file for Figure 10 (WS1) and its corresponding output file. This model simulates a target waste storage array of 180 ²³⁵U-water spheres (4.0L each) on a square pitch in a fully flooded condition. This means the interstitial region between each sphere in the lattice is flooded with water, and an infinite water reflector surrounds the entire external region of the array. Each sphere contains a homogenous mixture of 1.80 moles of ²³⁵U and 220 moles of water.

```
hot cell criticality calculation
c =====
c 2 X 9 X 10 array of unit spheres
c 1.8 moles U-235
c 220 moles water
c =====
c
c CELL CARDS
c
c U-235/water sphere
1 1 0.10047 -1 u=1 imp:n=1
c
c water moderator between spheres
2 2 -1.0 1 u=1 imp:n=1
c void between spheres
c 2 0 1 u=1 imp:n=1
c
c square lattice card
3 0 -10 20 -30 40 -50 60 lat=1 u=2 fill=1 imp:n=1
c
c bounding surfaces of array
4 0 -100 200 -300 400 -500 600 fill=2 imp:n=1
c
c 10 cm water reflector
5 2 -1.0 -110 120 -130 140 -150 160 #4 imp:n=1
c
c outside world
c bare configuration
c 6 0 100:-200:300:-400:500:-600 imp:n=0
c reflected configuration
6 0 110:-120:130:-140:150:-160 imp:n=0
c
c SURFACE CARDS
c
1 so 9.847 $U-235/water sphere
```

c
c lattice surfaces
10 px 37.247 \$x-bounding surface (right)
20 px -37.247 \$x-bounding surface (left)
30 py 30.477 \$y-bounding surface (above)
40 py -30.477 \$y-bounding surface (below)
50 pz 45.717 \$z-bounding surface (top of box)
60 pz -45.717 \$z-bounding surface (bottom of box)

c
c window surfaces just inside boundaries of lattice
100 px 707.80 \$x-window surface (right)
200 px -37.24 \$x-window surface (left)
300 py 518.14 \$y-window surface (above)
400 py -30.47 \$y-window surface (below)
500 pz 137.15 \$z-window surface (top of box)
600 pz -45.71 \$z-window surface (bottom of box)

c
c water reflector surfaces
110 px 717.80
120 px -47.24
130 py 528.14
140 py -40.47
150 pz 147.15
160 pz -55.71

c
c MATERIAL CARDS

c
kcode 1000 1.0 15 115
ksrc 0 0 0 670.5 0 0 0 426.72 0 670.5 426.72 0
223.5 121.92 0 447 121.92 0 223.5 304.8 0
447 304.8 0 0 0 91.44 670.5 0 91.44
0 426.72 91.44 670.5 426.72 91.44 223.5 121.92 91.44
447 121.92 91.44 223.5 304.8 91.44 447 304.8 91.44

c
c homogenous mixture of U-235 and water
m1 92235.50c 2.7337e-4 \$uranium-235
8016.50c 0.0334 \$oxygen
1001.50c 0.0668 \$hydrogen
mt1 lwtr.01t \$water T=300 K
c water moderator
m2 1001.50c 2.00 \$hydrogen
8016.50c 1.00 \$oxygen
mt2 lwtr.01t \$water T=300 K

k(collision) 0.811397 0.820635 0.0043 k(col/abs) 0.820456 0.0034 0.820384 0.0033 0.5040
k(absorption) 0.802914 0.820276 0.0035 k(abs/trk ln) 0.820405 0.0034 0.820357 0.0033 0.4910
k(trk length) 0.813021 0.820534 0.0043 k(tk ln/col) 0.820585 0.0043 0.820555 0.0043 0.9804
rem life(col) 1.2051E+04 1.2229E+04 0.0048 k(col/abs/trk ln) 0.820482 0.0036 0.820335 0.0033
rem life(abs) 1.2183E+04 1.2233E+04 0.0047 life(col/abs) 1.2231E+04 0.0047 1.2233E+04 0.0047
0.9807

source points generated 989

source distribution written to file srctp cycle = 115

1 problem summary

run terminated when 115 kcode cycles were done.

+

hot cell criticality calculation

04/09/98 14:19:00

probid = 04/09/98 13:21:59

0

neutron creation	tracks	weight	energy
(per source particle)			
source	115397	9.9656E-01	2.0345E+00
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	0	1.3751E-01	5.2365E-08
energy importance	0	0.	0.
dxtran	0	0.	0.
forced collisions	0	0.	0.
exp. transform	0	0.	0.
upscattering	0	0.	6.9693E-07
(n,xn)	4	2.6337E-05	1.0534E-05
fission	0	0.	0.
total	115401	1.1341E+00	2.0345E+00

neutron loss	tracks	weight	energy
(per source particle)			
escape	55	3.7627E-04	6.1428E-04
energy cutoff	0	0.	0.
time cutoff	0	0.	0.
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	115344	1.3692E-01	5.3648E-08
energy importance	0	0.	0.
dxtran	0	0.	0.
forced collisions	0	0.	0.
exp. transform	0	0.	0.
downscattering	0	0.	2.0128E+00
capture	0	6.6026E-01	1.7576E-02
loss to (n,xn)	2	1.3169E-05	9.6735E-05
loss to fission	0	3.3652E-01	3.4958E-03
total	115401	1.1341E+00	2.0345E+00

number of neutrons banked 2
neutron tracks per source particle 1.0000E+00
neutron collisions per source particle 2.1592E+02
total neutron collisions 24916200
net multiplication 1.0000E+00 0.0002

average lifetime, shakes
escape 4.1969E+03 tco 1.0000E+34
capture 1.2202E+04 eco 0.0000E+00
capture or escape 1.2199E+04 wc1 -5.0000E-01
any termination 1.5267E+04 wc2 -2.5000E-01

computer time so far in this run 57.02 minutes
computer time in mcrun 55.10 minutes
source particles per minute 2.0942E+03
random numbers generated 193794817

maximum number ever in bank 1
bank overflows to backup file 0
field length 0
most random numbers used was 15503 in history 84437

keff estimator	keff	standard deviation	68% confidence	95% confidence	99% confidence
collision	0.82064	0.00354	0.81710 to 0.82417	0.81359 to 0.82768	0.81130 to 0.829
absorption	0.82028	0.00288	0.81740 to 0.82316	0.81454 to 0.82601	0.81267 to 0.827
track length	0.82053	0.00349	0.81704 to 0.82403	0.81357 to 0.82750	0.81130 to 0.829
col/absorp	0.82038	0.00272	0.81766 to 0.82311	0.81496 to 0.82581	0.81319 to 0.827
abs/trk len	0.82036	0.00270	0.81765 to 0.82306	0.81497 to 0.82574	0.81322 to 0.827
col/trk len	0.82055	0.00351	0.81704 to 0.82407	0.81356 to 0.82755	0.81128 to 0.829
col/abs/trk len	0.82033	0.00271	0.81762 to 0.82305	0.81493 to 0.82574	0.81317 to 0.827

if the largest of each keff occurred on the next cycle, the keff results and 68, 95, and 99 percent confidence interval

keff estimator	keff	standard deviation	68% confidence	95% confidence	99% confidence
collision	0.82165	0.00364	0.81800 to 0.82530	0.81439 to 0.82891	0.81202 to 0.831
absorption	0.82097	0.00293	0.81804 to 0.82391	0.81513 to 0.82681	0.81322 to 0.828
track length	0.82153	0.00360	0.81793 to 0.82514	0.81436 to 0.82871	0.81202 to 0.831
col/abs/trk len	0.82110	0.00280	0.81830 to 0.82391	0.81553 to 0.82668	0.81371 to 0.828

the estimated collision/absorption neutron lifetimes, one standard deviations, and 68, 95, and 99 percent confidence in

type	lifetime(sec)	standard deviation	68% confidence	95% confidence	99% con
removal	1.2233E-04	5.7388E-07	1.2176E-04 to 1.2291E-04	1.2119E-04 to 1.2348E-04	1.2082E-04 t
capture	1.2220E-04	4.7465E-07	1.2173E-04 to 1.2268E-04	1.2126E-04 to 1.2315E-04	1.2095E-04 t
fission	4.3433E-05	2.2813E-07	4.3205E-05 to 4.3661E-05	4.2979E-05 to 4.3888E-05	4.2830E-05 t
escape	2.8493E-05	1.0187E-05	1.8295E-05 to 3.8691E-05	8.1994E-06 to 4.8786E-05	1.5775E-06 t

1 average individual and combined collision/absorption/track-length keff results for 7 different batch sizes

Storage Configuration WS3

The following is a sample MCNP input file for Figure 12 (WS3) and its corresponding output file. This model is for an array of 9 x 10 x 2 steel barrels each containing a hemisphere composed of a mixture of ^{235}U and water. To simulate a flooded condition, a 6-cm water reflector surrounds each hemisphere. The steel barrels are included in the model and are on a square pitch of 2.0 ft with one another. The array of barrels is surrounded by a concrete reflector to simulate the walls of Room 109. Each hemisphere is loaded with the maximum amount of fissile material allowed per barrel, 350 grams of ^{235}U .

```
hot cell criticality calculation
c =====
c 9 X 10 array of spheres
c 2.978 moles U-235
c 18.464 L water
c =====
c
c CELL CARDS
c
c void space between barrels
1 0 -6 7 -3 u=1 imp:n=1
c
c carbon steel caps on barrels
2 4 0.08586 -4 6 -3 u=1 imp:n=1 $bottom cap of top
barrel
3 4 0.08586 -7 5 -3 u=1 imp:n=1 $top cap of bottom
barrel
c
c
c U-235/water sphere
4 1 0.10029 -1 (3:4:-5) u=1 imp:n=1
c
c void space in water reflector
5 0 -6 7 1 -2 u=1 imp:n=1
c
c carbon steel caps on barrels
6 4 0.08586 -4 6 1 -2 u=1 imp:n=1 $bottom cap of
top barrel
7 4 0.08586 -7 5 1 -2 u=1 imp:n=1 $top cap of
bottom barrel
c
c water reflector outside sphere
8 2 -1.0 1 -2 #5 #6 #7 u=1 imp:n=1
c
c space between inside of barrel & sphere
9 0 2 -8 13 -11 u=1 imp:n=1
c
c carbon steel barrels (two barrels stacked axially)
```

```

10 4 0.08586 -12 14 -9 (8:11:-13) u=1 imp:n=1
c
c space outside barrel
11 0 -14:9:12 u=1 imp:n=1 $void
c 11 2 -1.0 -14:9:12 u=1 imp:n=1 $water
c
c square lattice card
12 0 -10 20 -30 40 -50 60 lat=1 u=2 fill=1 imp:n=1
c
c bounding surfaces of array
13 0 -100 200 -300 400 -500 600 fill=2 imp:n=1
c
c concrete reflector
14 3 -2.3 -110 120 -130 140 -150 160 #13 imp:n=1
c
c outside world
c bare configuration
c 9 0 100:-200:300:-400:500:-600 imp:n=0
c reflected configuration
15 0 110:-120:130:-140:150:-160 imp:n=0

c
c SURFACE CARDS
c
c U-235/water sphere
c 1 so 10.24
c 1 so 12.60
1 so 15.62
c 1 so 16.91
c 1 so 17.83
c 1 so 18.64
c 1 so 19.50
c 1 so 20.36
c
c 6 cm water reflector
c 2 so 16.24
c 2 so 18.60
2 so 21.62
c 2 so 22.91
c 2 so 23.83
c 2 so 24.64
c 2 so 25.50
c 2 so 26.36
c
c void space between barrels
c 3 cz 10.19
c 3 cz 12.56
3 cz 15.58
c 3 cz 16.88
c 3 cz 17.80

```

```

c 3      cz      18.61
c 3      cz      19.47
c 3      cz      20.33
4      pz      1.00
5      pz     -1.00
6      pz      0.86
7      pz     -0.86
c
8      cz      28.00      $inner radius of barrel from CL
9      cz      28.14      $outer radius of barrel from CL
11     pz      91.30      $inner height of top barrel cap from CL
12     pz      91.44      $outer height of top barrel cap from CL
13     pz     -91.299     $inner height of bottom barrel cap from
CL
14     pz     -91.439     $outer height of bottom barrel cap from
CL
c
c lattice surfaces (radial pitch 2.0 ft)
10     px      30.480     $x-bounding surface (right)
20     px     -30.480     $x-bounding surface (left)
30     py      30.480     $y-bounding surface (above)
40     py     -30.480     $y-bounding surface (below)
50     pz      182.880    $z-bounding surface (top of box, 6 ft from
CL)
60     pz     -91.440     $z-bounding surface (bottom of box, 3 ft
from CL)
c
c window surfaces for outer boundaries of lattice
100    px      579.11     $x-window surface (right)
200    px     -30.47     $x-window surface (left)
300    py      518.15     $y-window surface (above)
400    py     -30.47     $y-window surface (below)
500    pz      182.87     $z-window surface (top of box)
600    pz     -91.45     $z-window surface (bottom of box)
c
c concrete reflector surfaces
110    px      635.12     $east wall (56 cm thick)
120    px     -86.48     $west wall (56 cm thick)
130    py      614.16     $north wall (96 cm thick)
140    py     -126.48     $south wall (96 cm thick)
150    pz      278.88     $outer edge of roof (96 cm thick)
160    pz     -187.44     $bottom of floor (96 cm thick)

c
c MATERIAL CARDS
c
kcode 1000  1.0  15  115
ksrc      0.0   0.0  2.0  548.64  0.0  2.0
          0.0  487.68  2.0  548.64  487.68  2.0
          243.84 243.84  2.0  304.80 243.84  2.0

```

```

c
c homogenous mixture of U-235 and water
c
c sphere volume 3844 g water (1922 hemisphere)
c ml 92235.50c 4.664e-4 $uranium-235
c 8016.50c 0.0334 $oxygen
c 1001.50c 0.0668 $hydrogen
c mt1 lwtr.01t $water T=300 K
c
c sphere volume 7390 g water (3695 hemisphere)
c ml 92235.50c 2.426e-4 $uranium-235
c 8016.50c 0.0334 $oxygen
c 1001.50c 0.0668 $hydrogen
c mt1 lwtr.01t $water T=300 K
c
c sphere volume 14432 g water (7216 hemisphere)
ml 92235.50c 1.242e-4 $uranium-235
8016.50c 0.0334 $oxygen
1001.50c 0.0668 $hydrogen
mt1 lwtr.01t $water T=300 K
c
c sphere volume 18464 g water (9232 hemisphere)
c ml 92235.50c 9.711e-5 $uranium-235
c 8016.50c 0.0334 $oxygen
c 1001.50c 0.0668 $hydrogen
c mt1 lwtr.01t $water T=300 K
c
c sphere volume 21738 g water (10869 hemisphere)
c ml 92235.50c 8.248e-5 $uranium-235
c 8016.50c 0.0334 $oxygen
c 1001.50c 0.0668 $hydrogen
c mt1 lwtr.01t $water T=300 K
c
c sphere volume 24938 g water (12469 hemisphere)
c ml 92235.50c 7.189e-5 $uranium-235
c 8016.50c 0.0334 $oxygen
c 1001.50c 0.0668 $hydrogen
c mt1 lwtr.01t $water T=300 K
c
c sphere volume 28662 g water (14331 hemisphere)
c ml 92235.50c 6.255e-5 $uranium-235
c 8016.50c 0.0334 $oxygen
c 1001.50c 0.0668 $hydrogen
c mt1 lwtr.01t $water T=300 K
c
c sphere volume 32756 g water (16378 hemisphere)
c ml 92235.50c 5.473e-5 $uranium-235
c 8016.50c 0.0334 $oxygen
c 1001.50c 0.0668 $hydrogen
c mt1 lwtr.01t $water T=300 K

```

```

c
c
c water moderator (1.0 g/cc)
m2      1001.50c      2.00      $hydrogen
        8016.50c      1.00      $oxygen
mt2     lwtr.01t      $water T=300 K
c
c concrete (KENO mixture, 2.3 g/cc)
m3      1001.50c      -0.010    $hydrogen
        8016.50c      -0.532    $oxygen
        14000.50c     -0.337    $silicon
        13027.50c     -0.034    $aluminum
        11023.50c     -0.029    $sodium
        20000.50c     -0.044    $calcium
        26000.50c     -0.014    $iron
c
c carbon steel (7.82 g/cc)
m4      26000.50c     0.0839    $iron
        12000.50c     0.00196   $carbon

```

```

=====
=====

```

```

estimator cycle 115 ave of 100 cycles combination simple average combined average corr
k(collision) 0.969989 0.911042 0.0042 k(col/abs) 0.911434 0.0031 0.911583 0.0029 0.3276
k(absorption) 0.966958 0.911826 0.0032 k(abs/TK ln) 0.911762 0.0031 0.911788 0.0029 0.3106
k(trk length) 0.970740 0.911698 0.0043 k(tk ln/col) 0.911370 0.0043 0.910721 0.0043 0.9908
rem life(col) 3.9771E+04 4.2494E+04 0.0096 k(col/abs/TK ln) 0.911522 0.0033 0.911691 0.0030
rem life(abs) 4.0054E+04 4.2520E+04 0.0096 life(col/abs) 4.2507E+04 0.0096 4.2519E+04 0.0096
0.9929

```

source points generated 1122

source distribution written to file srctp cycle = 115
1 problem summary

run terminated when 115 kcode cycles were done.

+ hot cell criticality calculation

06/05/98 23:33:17
probid = 06/05/98 21:46:48

neutron creation				neutron loss			
tracks	weight	energy	tracks	weight	energy		
(per source particle)			(per source particle)				
source	115760	9.9343E-01	2.0349E+00	escape	156	6.0149E-04	1.0454E-04
weight window	0	0.	0.	energy cutoff	0	0.	0.
cell importance	0	0.	0.	time cutoff	0	0.	0.
weight cutoff	0	1.0874E-01	3.9956E-08	weight window	0	0.	0.
energy importance	0	0.	0.	cell importance	0	0.	0.
dextran	0	0.	0.	weight cutoff	115604	1.0936E-01	2.7565E-05
forced collisions	0	0.	0.	energy importance	0	0.	0.
exp. transform	0	0.	0.	dextran	0	0.	0.
upscattering	0	0.	4.5051E-07	forced collisions	0	0.	0.
(n,xn)	0	0.	0.	exp. transform	0	0.	0.
fission	0	0.	0.	downscattering	0	0.	2.0069E+00
total	115760	1.1022E+00	2.0349E+00	capture	0	6.1946E-01	2.6020E-02
				loss to (n,xn)	0	0.	0.
				loss to fission	0	3.7276E-01	1.8057E-03
				total	115760	1.1022E+00	2.0349E+00

```

number of neutrons banked 0
neutron tracks per source particle 1.0000E+00
neutron collisions per source particle 1.2451E+02
total neutron collisions 14413394
net multiplication 1.0000E+00 0.0002

```

```

average lifetime, shakes cutoffs
escape 9.5212E+04 tco 1.0000E+34
capture 4.2278E+04 eco 0.0000E+00
capture or escape 4.2310E+04 wc1 -5.0000E-01
any termination 5.5635E+04 wc2 -2.5000E-01

```

computer time so far in this run 106.48 minutes maximum number ever in bank 0
 computer time in mcrun 102.23 minutes bank overflows to backup file 0
 source particles per minute 1.1323E+03 field length 0
 random numbers generated 160461760 most random numbers used was 13081 in history 63834

keff estimator	keff	standard deviation	68% confidence	95% confidence	99% confidence
collision	0.91104	0.00385	0.90719 to 0.91489	0.90338 to 0.91870	0.90088 to 0.921
absorption	0.91183	0.00295	0.90888 to 0.91478	0.90595 to 0.91770	0.90404 to 0.919
track length	0.91170	0.00392	0.90778 to 0.91562	0.90389 to 0.91950	0.90135 to 0.922
col/absorp	0.91158	0.00269	0.90889 to 0.91427	0.90623 to 0.91694	0.90448 to 0.918
abs/trk len	0.91179	0.00269	0.90910 to 0.91448	0.90644 to 0.91714	0.90469 to 0.918
col/trk len	0.91072	0.00389	0.90683 to 0.91461	0.90298 to 0.91846	0.90045 to 0.920
col/abs/trk len	0.91169	0.00272	0.90897 to 0.91442	0.90627 to 0.91711	0.90450 to 0.918

if the largest of each keff occurred on the next cycle, the keff results and 68, 95, and 99 percent confidence interval

keff estimator	keff	standard deviation	68% confidence	95% confidence	99% confidence
collision	0.91197	0.00392	0.90805 to 0.91589	0.90416 to 0.91978	0.90161 to 0.922
absorption	0.91244	0.00298	0.90946 to 0.91543	0.90650 to 0.91838	0.90456 to 0.920
track length	0.91263	0.00399	0.90864 to 0.91662	0.90468 to 0.92058	0.90209 to 0.923
col/abs/trk len	0.91241	0.00279	0.90962 to 0.91521	0.90686 to 0.91797	0.90504 to 0.919

the estimated collision/absorption neutron lifetimes, one standard deviations, and 68, 95, and 99 percent confidence in

type	lifetime(sec)	standard deviation	68% confidence	95% confidence	99% con
removal	4.2519E-04	4.0973E-06	4.2109E-04 to 4.2930E-04	4.1703E-04 to 4.3336E-04	4.1437E-04 t
capture	4.2500E-04	3.8908E-06	4.2110E-04 to 4.2889E-04	4.1725E-04 to 4.3275E-04	4.1472E-04 t
fission	6.3230E-05	5.3771E-07	6.2692E-05 to 6.3768E-05	6.2159E-05 to 6.4301E-05	6.1810E-05 t
escape	8.3577E-04	9.4191E-05	7.4149E-04 to 9.3006E-04	6.4814E-04 to 1.0234E-03	5.8692E-04 t

1 average individual and combined collision/absorption/track-length keff results for 7 different batch sizes

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Appendix C Sample Calculations

Target Atom Density Calculation

Given parameters: 36.65 grams UO_2
 93 w/o ^{235}U in UO_2
 stainless steel cladding 25 mils thick (0.0635 cm)
 3.175 cm (1.25 in.) target diameter
 41.91 cm (16.5 in.) UO_2 fuel height
 2.803 cm^3 UO_2 per target

This calculation summarizes the algorithm used to obtain the atom densities for input into MCNP for a target coated with 36.65 grams of uranium dioxide (UO_2). Based on the ^{235}U enrichment of the target, the average atomic weight of uranium (U) in the UO_2 is calculated as follows:

$$\bar{M}_U = \left[\frac{wf_{235}}{M_{235}} + \frac{wf_{238}}{M_{238}} \right]^{-1} = \left[\frac{0.97}{235.044} + \frac{0.07}{238.051} \right]^{-1} = 235.252 \text{ grams } U$$

Translating this to the average molecular weight of UO_2 in the target by including the oxygen (O) gives,

$$\bar{M}_{UO_2} = 235.252 \text{ g } U + 2(16.0 \text{ g } O) = 267.252 \text{ grams } UO_2$$

Before calculating the atom densities of ^{235}U and ^{238}U , the atom densities of uranium and oxygen must be derived. In general, the atom density of a material is defined as,

$$N = \frac{\rho * N_A}{M}$$

where ρ is the density of the material, N_A is Avogadro's number, and M is the atomic weight of the material. So the mass per unit volume or density of UO_2 molecules in the target layer is found by dividing the mass of the UO_2 in the target by its respective volume,

$$\rho_{UO_2} = \frac{M_{UO_2}}{V_{UO_2}} = \frac{36.65 \text{ g } UO_2}{2.803 \text{ cm}^3} = 13.08 \frac{\text{grams } UO_2}{\text{cm}^3}$$

Therefore, the atom density, or more appropriately molecular density of UO_2 in this case is,

$$N_{\text{UO}_2} = \frac{\rho_{\text{UO}_2} * N_A}{M_{\text{UO}_2}} = \left(\frac{13.08 \text{ g UO}_2}{\text{cm}^3} \right) \left(\frac{6.022 \times 10^{23} \text{ molec UO}_2}{\text{mol UO}_2} \right) \left(\frac{\text{mol UO}_2}{267.252 \text{ g UO}_2} \right)$$

$$N_{\text{UO}_2} = 2.947 \times 10^{22} \frac{\text{molec UO}_2}{\text{cm}^3}$$

The atom densities of uranium and oxygen are determined by using the molecular structure of UO₂ in the calculation as follows:

$$N_U = af_U * N_{\text{UO}_2} = \left(\frac{1 \text{ atom U}}{\text{molec UO}_2} \right) \left(\frac{2.947 \times 10^{22} \text{ molec UO}_2}{\text{cm}^3} \right)$$

$$N_U = 2.947 \times 10^{22} \frac{\text{atoms U}}{\text{cm}^3}$$

$$N_O = af_O * N_{\text{UO}_2} = \left(\frac{2 \text{ atoms O}}{\text{molec UO}_2} \right) \left(\frac{2.947 \times 10^{22} \text{ molec UO}_2}{\text{cm}^3} \right)$$

$$N_O = 5.893 \times 10^{22} \frac{\text{atoms O}}{\text{cm}^3}$$

where af is the atom fraction or number of uranium and oxygen atoms composing the UO₂ molecule. To determine the atom densities of ²³⁵U, ²³⁸U, and oxygen, the respective atom fractions of each must be determined by the following equation:

$$af_i = wf_i \left(\frac{\bar{M}_U}{M_i} \right)$$

where wf_i is the weight fraction of i^{th} material, \bar{M}_U is the average atomic weight of uranium in the UO₂, and M_i is the atomic weight of the i^{th} material. Calculating the atom fractions of ²³⁵U and ²³⁸U based on the ²³⁵U enrichment for this problem yields:

$$af_{235} = wf_{235} \left(\frac{\bar{M}_U}{M_{235}} \right) = \left(\frac{0.93 \text{ atoms } ^{235}\text{U}}{\text{atoms U}} \right) \left(\frac{235.252 \text{ grams U}}{235.044 \text{ grams } ^{235}\text{U}} \right)$$

$$af_{235} = 0.9308 \frac{\text{atoms } ^{235}\text{U}}{\text{atoms U}}$$

$$af_{238} = wf_{238} \left(\frac{\bar{M}_U}{M_{238}} \right) = \left(\frac{0.07 \text{ atoms } ^{238}\text{U}}{\text{atoms U}} \right) \left(\frac{235.252 \text{ grams U}}{238.051 \text{ grams } ^{238}\text{U}} \right)$$

$$af_{238} = 0.0692 \frac{\text{atoms } ^{238}\text{U}}{\text{atoms U}}$$

Using these atom fractions, the atom densities of ^{235}U , ^{238}U , and oxygen can now be determined. They must be calculated in units of atoms/b-cm for input into MCNP.

$$N_{235} = af_{235} * N_U = \left(\frac{0.9308 \text{ atoms } ^{235}\text{U}}{\text{atoms U}} \right) \left(\frac{2.947 \times 10^{22} \text{ atoms U}}{\text{cm}^3} \right) \left(\frac{10^{-24} \text{ cm}^2}{b} \right)$$

$$N_{235} = 0.02743 \frac{\text{atoms } ^{235}\text{U}}{b - \text{cm}}$$

$$N_{238} = af_{238} * N_U = \left(\frac{0.0692 \text{ atoms } ^{238}\text{U}}{\text{atoms U}} \right) \left(\frac{2.947 \times 10^{22} \text{ atoms U}}{\text{cm}^3} \right) \left(\frac{10^{-24} \text{ cm}^2}{b} \right)$$

$$N_{238} = 0.00204 \frac{\text{atoms } ^{238}\text{U}}{b - \text{cm}}$$

$$N_O = \left(\frac{5.893 \times 10^{22} \text{ atoms O}}{\text{cm}^3} \right) \left(\frac{10^{-24} \text{ cm}^2}{b} \right)$$

$$N_O = 0.05893 \frac{\text{atoms O}}{b - \text{cm}}$$

Finally, the atom density of ^{235}U and the volume of the UO_2 layer in the target are used to obtain the mass of ^{235}U in the target coating.

$$m_{235} = \frac{N_{235} * V_{\text{UO}_2} * M_{235}}{N_A}$$

$$m_{235} = \left(\frac{2.947 \times 10^{22} \text{ atoms } ^{235}\text{U}}{\text{cm}^3 \text{ UO}_2} \right) \left(\frac{2.803 \text{ cm}^3 \text{ UO}_2}{\text{target}} \right) \left(\frac{\text{mol } ^{235}\text{U}}{6.022 \times 10^{23} \text{ atoms } ^{235}\text{U}} \right) \left(\frac{235.044 \text{ grams } ^{235}\text{U}}{\text{mol } ^{235}\text{U}} \right)$$

$$\therefore m_{235} = 30.00 \frac{\text{grams } ^{235}\text{U}}{\text{target}}$$

Waste Storage Atom Density Calculations

This set of sample calculations explains how the atom densities were derived for the waste storage configurations WS1 and WS3 for input into MCNP.

Storage Configuration WS1

Given parameters: square lattice array of 180 4.0L spheres of $^{235}\text{U}-\text{H}_2\text{O}$
 1.80 moles of ^{235}U per sphere
 external water reflector

To obtain the density of water in the ^{235}U -water mixture of each sphere, the mass of the water must be converted from moles to grams.

$$m_{\text{water}} = (220 \text{ mol } \text{H}_2\text{O}) \left(\frac{18.0 \text{ g } \text{H}_2\text{O}}{\text{mol } \text{H}_2\text{O}} \right) = 3960 \text{ grams } \text{H}_2\text{O}$$

$$\rho_{\text{water}} = \frac{3960 \text{ grams } \text{H}_2\text{O}}{4000 \text{ cm}^3 \text{ H}_2\text{O}} = 0.99 \text{ g / cm}^3$$

Since the resulting density of water is close to the theoretical value, then it is assumed each 4.0-L sphere is completely saturated with water. Using this density value, the atom density of each constituent of the mixture can be found. For input into MCNP, each is derived in units of atoms/b-cm. First, the water molecular density can be found as follows,

$$N_{\text{water}} = \frac{\rho * N_A}{M_{\text{water}}} = \left(\frac{0.99 \text{ g}}{\text{cm}^3} \right) \left(\frac{\text{mol } \text{H}_2\text{O}}{18 \text{ g } \text{H}_2\text{O}} \right) \left(\frac{6.022 \times 10^{23} \text{ molec } \text{H}_2\text{O}}{\text{mol } \text{H}_2\text{O}} \right)$$

$$N_{\text{water}} = 0.0334 \frac{\text{molec } \text{H}_2\text{O}}{\text{b-cm}}$$

Based on the molecular density of water in the mixture, the atom densities of the hydrogen and oxygen are derived as follows,

$$N_H = a f_H * N_{\text{water}} = \left(\frac{2 \text{ atoms } \text{H}}{\text{molec } \text{H}_2\text{O}} \right) \left(\frac{0.0334 \text{ molec } \text{H}_2\text{O}}{\text{b-cm}} \right)$$

$$N_H = 0.0668 \frac{\text{atoms } \text{H}}{\text{b-cm}}$$

$$N_O = af_o * N_{water} = \left(\frac{1 \text{ atom O}}{\text{molec H}_2\text{O}} \right) \left(\frac{0.0334 \text{ molec H}_2\text{O}}{b - cm} \right)$$

$$N_O = 0.0334 \frac{\text{atoms O}}{b - cm}$$

These atom densities are close to those for hydrogen and oxygen in nominal water since the majority of the mixture is composed of water and the density is close to the theoretical value. Now the atom density of ^{235}U in the mixture can be found based on its mass in the mixture as follows,

$$N_{235} = \frac{m_{235} * N_A}{V_{water}} = \left(\frac{1.80 \text{ mol } ^{235}\text{U}}{3960 \text{ cm}^3 \text{ H}_2\text{O}} \right) \left(\frac{6.022 \times 10^{23} \text{ atoms } ^{235}\text{U}}{\text{mol } ^{235}\text{U}} \right) \left(\frac{10^{-24} \text{ cm}^2}{b} \right)$$

$$N_{235} = 2.7372 \times 10^{-4} \frac{\text{atoms } ^{235}\text{U}}{b - cm}$$

The H / ^{235}U ratio is a parameter commonly used in criticality safety studies to quantify the degree of moderation for a particular system. In this case, it is found by dividing the atom density of hydrogen in the mixture of a sphere by the atom density of ^{235}U in the same sphere. The following is the H / ^{235}U ratio for the sample model of 180 4.0 L spheres.

$$\frac{H}{^{235}\text{U}} = \frac{N_H}{N_{U235}} = \frac{6.68 \times 10^{-2} \frac{\text{atoms H}}{b - cm}}{2.7372 \times 10^{-4} \frac{\text{atoms } ^{235}\text{U}}{b - cm}} = 244$$

Storage Configuration WS3

Given parameters: square lattice array of 180 barrels (one ^{235}U -H₂O hemisphere per barrel)
 7,216 cm³ hemisphere
 350 grams ^{235}U per hemisphere
 6 cm external water reflector on each hemisphere

This storage configuration was modeled with the MCNP and KENO codes. Unlike KENO, MCNP lacks the capability to model hemispheres explicitly and this configuration was instead modeled as 90 spheres. To maintain geometric consistency with the hemispheres modeled in KENO, a void space was introduced at the center of each sphere. This was done to make the spheres into pseudo-hemispheres, and to simulate the void space at the barrel interfaces as shown in Figure 12 (WS3).

This study consisted of calculating the k_{eff} for a variety of H / ^{235}U ratios. This entailed keeping the ^{235}U mass constant while varying the water volume, and ultimately the sphere volume. Each sphere contained 700 grams of ^{235}U , or 350 grams per hemisphere which is the maximum

allowed per barrel. First, to derive the atom densities of ^{235}U , hydrogen, and oxygen in the mixture for input into the code, the number of atoms of ^{235}U and water in the mixture must be calculated as follows:

$$n_{235} = m_{235} * N_A = (2.978 \text{ mol } ^{235}\text{U}) \left(\frac{6.022 \times 10^{23} \text{ atoms } ^{235}\text{U}}{\text{mol } ^{235}\text{U}} \right)$$

$$n_{235} = 1.793 \times 10^{24} \text{ atoms } ^{235}\text{U}$$

$$n_{\text{water}} = \frac{m_{\text{water}} * N_A}{M_{\text{water}}} = (14432 \text{ g } H_2O) \left(\frac{\text{mol } H_2O}{18 \text{ g } H_2O} \right) \left(\frac{6.022 \times 10^{23} \text{ molec } H_2O}{\text{mol } H_2O} \right)$$

$$n_{\text{water}} = 4.828 \times 10^{26} \text{ molec } H_2O$$

It is assumed that the water in the ^{235}U -water mixture is of theoretical density, 1.0 g/cm^3 . Consequently, the number of hydrogen and oxygen atoms can be calculated as,

$$n_H = n_{\text{water}} * af_H = (4.828 \times 10^{26} \text{ molec } H_2O) \left(\frac{2 \text{ atoms } H}{\text{molec } H_2O} \right)$$

$$n_H = 9.656 \times 10^{26} \text{ atoms } H$$

$$n_O = n_{\text{water}} * af_O = (4.828 \times 10^{26} \text{ molec } H_2O) \left(\frac{1 \text{ atoms } O}{\text{molec } H_2O} \right)$$

$$n_O = 4.828 \times 10^{26} \text{ atoms } O$$

Now, the atom densities of ^{235}U , hydrogen, and oxygen are derived by dividing the number of atoms into the sphere volume and converting to units of atoms/b-cm.

$$N_{235} = \frac{n_{235}}{V_{\text{sph}}} = \left(\frac{1.793 \times 10^{24} \text{ atoms } ^{235}\text{U}}{14432 \text{ cm}^3} \right) \left(\frac{10^{-24} \text{ cm}^2}{b} \right)$$

$$N_{235} = 1.242 \times 10^{-4} \frac{\text{atoms } ^{235}\text{U}}{b - \text{cm}}$$

$$N_H = \frac{n_H}{V_{\text{sph}}} = \left(\frac{9.656 \times 10^{26} \text{ atoms } H}{14432 \text{ cm}^3} \right) \left(\frac{10^{-24} \text{ cm}^2}{b} \right)$$

$$N_H = 0.0669 \frac{\text{atoms } H}{b - \text{cm}}$$

$$N_o = \frac{n_o}{V_{sph}} = \left(\frac{4.828 \times 10^{26} \text{ atoms } O}{14432 \text{ cm}^3} \right) \left(\frac{10^{-24} \text{ cm}^2}{b} \right)$$

$$N_o = 0.0335 \frac{\text{atoms } O}{b - \text{cm}}$$

The H / ²³⁵U ratio was calculated by dividing the number of hydrogen atoms into the number of ²³⁵U atoms as follows.

$$\frac{H}{^{235}\text{U}} = \frac{n_H}{n_{U^{235}}} = \frac{4.828 \times 10^{26} \text{ atoms } H}{1.793 \times 10^{24} \text{ atoms } ^{235}\text{U}} = 539$$

This entire procedure was repeated for a variety of sphere volumes in order to calculate the k_{eff} for a range of H / ²³⁵U ratios.

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