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Bounding Pressure and Flammability Evaluations for a Department of Energy Standard Canister Loaded with Aluminum-Clad Spent Fuel

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SUMMARY

This report presents bounding pressurization and flammability evaluations from the radiolytic gas generation expected during extended (>50 years) dry storage of aluminum-clad spent nuclear fuel (ASNF) elements in a sealed Department of Energy (DOE) Standard Canister. The primary questions involving extended ASNF dry storage center around the adequacy of dry storage conditioning processes (i.e., drying) and the behavior of residual hydrated aluminum oxides on the cladding—specifically, the radiolytic breakdown of chemically bound water in these corrosion products. The objectives of the presented work include providing a bounding assessment of the pressure with respect to the DOE Standard Canister's structural integrity limits and identifying the potential for forming flammable or explosive gas mixtures (i.e., exceedance of the lower flammability limit of the molecular hydrogen [H_2] and oxygen [O_2] concentrations).

Recent structural evaluations of the DOE Standard Canister determined a structural canister pressure limit of 3,447 kPag (500 psig) at room temperature. This structural limit can be compared to 2007 bounding pressure estimates in a DOE Standard Canister loaded with Advanced Test Reactor (ATR) ASNF utilizing Type 1a baskets. This ASNF type has a high decay heat and dose rate, which could promote radiolytic gas generation and subsequent canister pressurization. Further, it has a high ratio of ASNF surface area-to-void volume, and thus, should present a bounding case for canister pressurization. The 2007 estimates considered highly conservative assumptions, such as that all water is radiolytically broken down and all available hydrogen is released into the canister atmosphere as H_2. Even under these conservative assumptions, the maximum calculated pressure in this configuration remained well below the structural limit of the DOE Standard Canister.

Recently, new DOE Standard Canister ASNF loading configurations were proposed and analyzed for fit and criticality. These design updates required an update of the existing bounding pressure calculations, and relevant preliminary evaluations were initiated. Ultimately, the results of these 2022 evaluations served for validation and verification purposes of more complex modeling and simulation (M&S) efforts. This M&S work was conducted within the DOE Office of Environmental Management Spent Nuclear Fuel (SNF) Technology Development project to address issues related to managing, storing, transporting, and disposing of DOE-managed SNF.

Since then, additional research was completed, building more confidence in a credible range of pressure controlling parameters, such as the thickness of the oxide layer adherent to the ASNF. Further, researchers confirmed the absence of oxygen—one of the key chemical species for establishing a flammable atmosphere—in helium-backfilled ASNF dry storage configurations. Furthermore, the computational fluid dynamics computation of considered DOE Standard Canister dry storage configurations provided lower estimates for realistic upper limit canister cover gas temperatures. These new insights, combined with refined geometrical parameter estimates, such as the DOE Standard Canister void volume, allow for more credible upper bound pressure calculations. Additionally, structural evaluations of the canister pressure structural limit at elevated temperatures under normal conditions enable the

comparison of these refined estimates with pressure limits computed according to the applicable codes (i.e., The American Society for Mechanical Engineers, Boiler and Pressure Vessel Code Section III – Rules for Construction of Nuclear Facility Components – Division 3 – Containment Systems & Transport Packagings for Spent Nuclear Fuel & High Level Radioactive Waste).

The evaluations in this report focused on two configurations: (1) dry storage in a ~10ft long, 18in. diameter (10 × 18) DOE Standard Canister capable of accommodating 32 individual ATR ASNF elements; and (2), dry storage in a ~10ft long, 24in. diameter (10 × 24) DOE Standard Canister capable of accommodating 40 individual ATR ASNF elements. A trihydrate (gibbsite, bayerite, i.e., $Al_2O_3 \bullet 3H_2O$) oxide layer is assumed to adhere to the surface of the ASNF ATR elements. This is a conservative assumption considering the higher water content of trihydrate compared to monohydrate (boehmite, i.e., $Al_2O_3 \bullet H_2O$). Thus, the complete radiolytic breakdown of trihydrate could lead to a release of more H_2 than the breakdown of monohydrate. However, ASNF drying experiments point to a possible phase transition of trihydrates to monohydrates at high drying temperatures (>220°C), demonstrating the benefits of high-temperature drying methods (such as forced helium dehydration) on ASNF dry storage safety.

The evaluation results confirm the findings of previous, more complex M&S work. That is, the structural integrity of the canister remains unchallenged by a wide margin. Nevertheless, it is important to recognize that the presented pressure calculations consider a full breakdown of the chemisorbed water, including a consequent release of all available H_2. In reality, the breakdown of water in these systems will likely remain incomplete, due to competing chemical and radiolytic reactions, thereby attaining an equilibrium in the storage environment.

In addition to the pressure calculations, a computation of the H_2 and O_2 concentration for selected cases was completed, providing insights into the possible gas mixture compositions. Similar to the assumptions made for the pressure calculations, all available water was assumed to break down, and all available H_2 was assumed to be released. Further, hypothetical cases of oxyhydrogen generation from radiolytic breakdown of residual steam and free water were evaluated. Under this assumption, the H_2 concentration exceeded the lower flammability limit of 4%; however, controlling the O_2 content (i.e., keeping it below 4%) ensures that flammable or explosive mixtures do not occur.

Lastly, sensitivity studies on selected parameters allowed for the identification of important pressure and flammability controlling parameters (i.e., the free void volume of the canister, oxide layer thickness and associated properties, and gas and canister material temperatures). Thus, it is important to recognize the importance of these parameters on ASNF dry storage safety in future configuration designs.

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FIGURES

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ACRONYMS

ASME	American Society for Mechanical Engineers
ASNF	aluminum-clad spent nuclear fuel
ATR	Advanced Test Reactor
BPVC	Boiler and Pressure Vessel Code
CFD	computational fluid dynamics
CRWMS	Civilian Radioactive Waste Management System
DOE	Department of Energy
INL	Idaho National Laboratory
LFL	lower flammability limits
M&S	modeling and simulation
SCPE	Standard Canister Pressure Estimator
SNF	spent nuclear fuel

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Bounding Pressure and Flammability Evaluations for a Department of Energy Standard Canister Loaded with Aluminum-Clad Spent Fuel

1. INTRODUCTION

The U.S. Department of Energy (DOE) manages a range of spent nuclear fuel (SNF) types and must continue to safely manage these materials for an extended period of time. This SNF comes from a wide variety of reactor types, such as light- and heavy-water-moderated reactors, graphite-moderated reactors, and breeder reactors, with various cladding materials and enrichments. Aluminum-clad spent nuclear fuel[a] (ASNF) comprises nearly 10% of the total DOE-managed SNF units, weighing in at over 13 metric tons of heavy metal. Further, DOE operates two reactors that continue to generate ASNF.

DOE ASNF is either stored wet or dry. Currently, much of the DOE-managed ASNF is in vented dry storage configurations at Idaho National Laboratory's (INL's) CPP-603 facility, but ongoing DOE initiatives could move some of this ASNF into sealed dry storage configurations. Sealed ASNF dry storage comes with a range of technical and scientific challenges. Most importantly, ASNF cladding is more suspectable to corrosion than other nuclear fuel cladding types. These aluminum corrosion products (i.e., aluminum oxides, such as a mixture of boehmite monohydrates [$Al_2O_3 \cdot H_2O$] and gibbsite and bayerite trihydrates [$Al_2O_3 \cdot 3H_2O$]) could carry a significant amount of chemisorbed water. Due to the radiolytic gas generation processes occurring in water exposed to strong gamma radiation fields (Parker Quaife et al. 2020 and Conrad et al. 2022), there are concerns that any residual water within a dry storage canister could be broken down and that molecular hydrogen (H_2) (among other chemical species) could be released. Eventually, radiolytic gas generation could increase the internal pressure of a sealed dry storage canister, and/or exceed flammability limits.

This report provides pressure estimations and flammability evaluations of potential configurations for the dry storage of DOE-managed ASNF. These include 32 or 40 individual Advanced Test Reactor (ATR) ASNF elements in ATR4 buckets loaded into either 10 ft long, 18 in. diameter (10 × 18) or 10 ft long, 24 in. diameter (10 × 24) DOE Standard Canisters, respectively. To achieve a bounding state of these evaluations, highly conservative assumptions—such as a full radiolytic breakdown of all chemisorbed, physisorbed, and free water—are used. For assessing the structural canister integrity, the estimated pressure is compared to the permissible pressure computed according to the American Society for Mechanical Engineers (ASME), Boiler and Pressure Vessel Code (BPVC) Section III – Rules for Construction of Nuclear Facility Components – Division 3 – Containment Systems & Transport Packagings for Spent Nuclear Fuel & High Level Radioactive Waste. To assess canister flammability, the estimated H_2 and molecular oxygen (O_2) concentrations are compared to the lower flammability limit established in the literature.

Further, sensitivity studies are presented to identify pressure and flammability controlling parameters.

2. OBJECTIVES

The objectives of the presented work are:

1. Computing credible, conservative, upper bound pressure values in currently considered DOE Standard Canister ASNF dry storage configurations.
2. Evaluating flammability of the canister atmosphere in these configurations.
3. Identifying pressure or flammability controlling parameters for these configurations.

[a]Not all SNF made of aluminum is considered ASNF. Historically, ASNF refers to SNF comprised of aluminum plates.

2.1 Limitations

The objectives of the presented work and the interpretations of the associated results and findings are to define a credible, conservative, upper bound pressure and H_2 and O_2 concentrations to confirm previous findings on the safety and technical feasibility of extended dry storage of ASNF. This report is not meant to challenge or relax previously defined design specifications of the DOE Standard Canister which may or may not be more restrictive than the assumptions made in the present evaluations. No definite conclusions about the safety and technical feasibility of currently considered ASNF dry storage configurations can be made based on the findings of this limited work scope. A comprehensive assessment of ASNF dry storage safety and technical feasibility requires a review of existing or completion of additional structural, criticality, and shielding evaluations, among other safety-relevant activities. Specifically, the material interactions associated with long-term storage in a sealed canister would need to be reviewed and examined in greater detail. For instance, pressure and temperature are inextricably linked. Assumptions on the canister thermal conditions directly impact the appropriate level of conservatism because reaction rates, equilibrium behavior, and selected material properties are strongly temperature dependent. Further, the scope of the presented work is constrained by the operational details of the envisioned ASNF dry storage concepts, which may be subject to change in the future. Furthermore, the findings of the present study are products of compounding conservatisms, with parameter values being selected in a deterministic manner. Utilizing probabilistic parameter selection methods (e.g., utilizing established Monte Carlo methods) could greatly impact the quality and accuracy of the presented results and findings.

3. CONSIDERED ALUMINUM-CLAD SPENT NUCLEAR FUEL DRY STORAGE CONFIGURATION

This preliminary analysis considers ATR ASNF elements loaded in either a 10 × 18 DOE Standard Canister or a 10 × 24 DOE Standard Canister. In these configurations, ATR4 buckets—each bucket providing space for four ATR ASNF elements—within borated stainless steel dividers ("baskets") are used to hold the ATR elements. In both configurations, two baskets are stacked on top of each other, separated by a circular spacer disk. In the 10 × 18 canister configuration, each basket holds four ATR4 buckets for a total of eight buckets, providing a total canister capacity of 32 ATR ASNF elements. In the 10 × 24 canister configuration, each of the two baskets holds five ATR4 buckets for a total of 10 buckets, providing a total canister capacity of 40 ATR ASNF elements. Additional details on the considered configurations are in the following sections.

3.1 The Department of Energy Standard Canister

To enable extended storage (>50 years) of a range of DOE-managed SNF, a sealed (i.e., leak tight) standardized canister system, termed the DOE Standard Canister, was proposed (Morton 1999) (see sketch in Figure 1). This robust, welded canister system is designed to confine radionuclides, to preclude content moderation, and to satisfy primary containment of SNF as part of an envisioned storage, transportation, and disposal system.

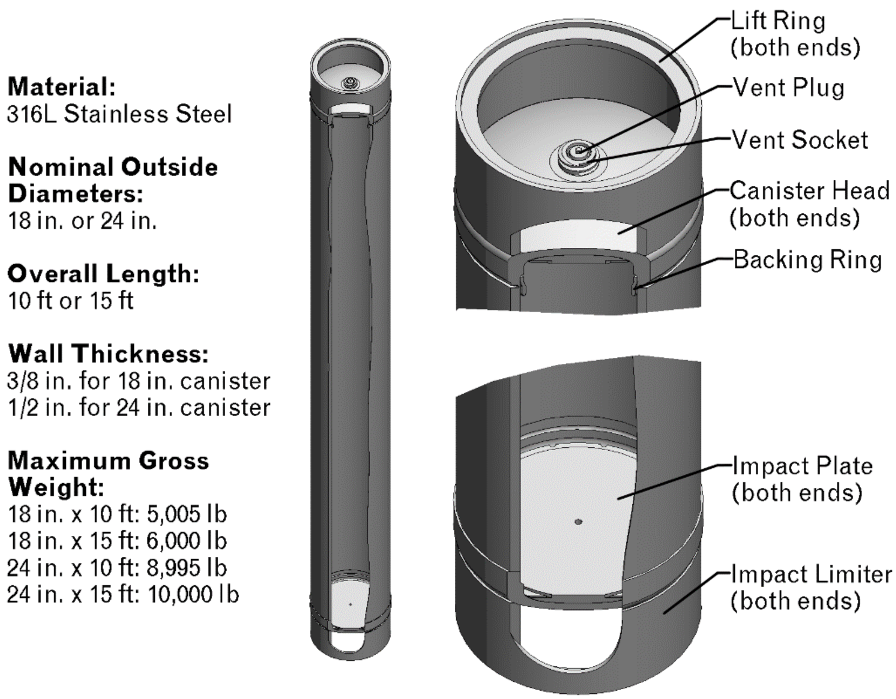

Figure 1. Sketch of the DOE Standard Canister design.

Each DOE Standard Canister is made of a right circular cylinder 316L stainless steel pipe with a welded torispherical bottom and top head. Currently, four versions of the design exist. Each version is distinguished by the outer diameter of the cylindrical canister shell (i.e., 18 and 24 in.) and the outer length of the canister (i.e., ~10 and 15 ft). The present evaluations consider the 10-ft-long designs (i.e., the 10 × 18 and 10 × 24 versions).

The 10 × 18 DOE Standard Canister shell has a wall thickness of 3/8 in., and the wall thickness of the torispherical head is 5/8 in. Recently completed three-dimensional modeling of three of the four DOE Standard Canister versions enables a computer-aided computation of the volume of the empty 10 × 18 canister cavity, which is 382,974 cm^3. No detailed drawings or three-dimensional computer models of the 10 × 24 canister version exist, but it is reasonable to assume a design similar to the 15 × 24 version. Thus, the 10 × 24 DOE Standard Canister considered in the present evaluations presumably has a shell wall thickness of 1/2 in. and a torispherical head wall thickness of 13/16 in. To estimate the volume of the empty 10 × 24 canister cavity, the assumption of a 10 × 24 canister cavity length equal to the 10 × 18 canister cavity length was made. Based on these assumptions the empty 10 × 24 DOE Standard Canister cavity volume is 660,416 cm^3.

3.2 Advanced Test Reactor Aluminum-Clad Spent Nuclear Fuel

The analyzed dry storage configurations are designed to accommodate 32 and 40 individual ATR ASNF elements within the 10 × 18 and 10 × 24 DOE Standard Canisters, respectively. Most of the existing ATR ASNF is currently in vented dry storage at INL's CPP-603 facility. A sketch of a typical ATR ASNF element is shown in Figure 2.

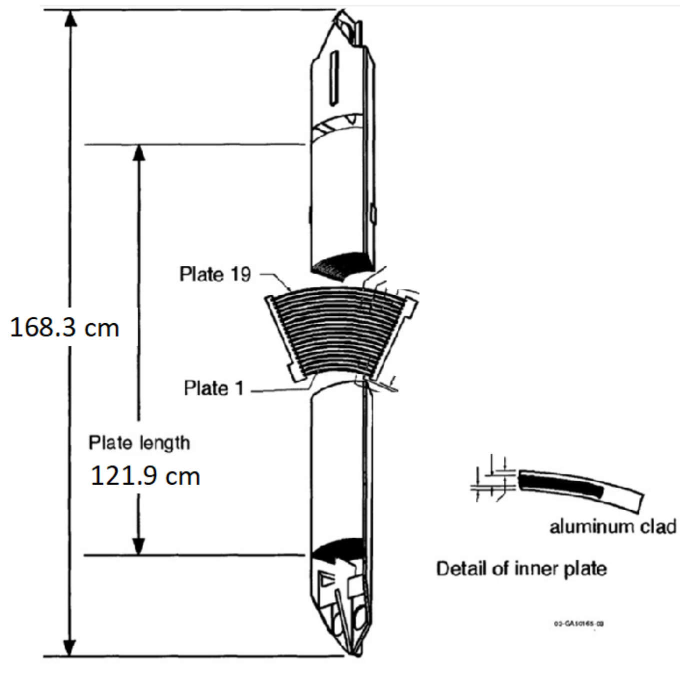

Figure 2. Typical ATR element.

A typical ATR fuel element has 19 curved aluminum-clad uranium aluminide plates. The design length of an ATR element is 168.3 cm; however, the upper and lower end boxes were chopped off from all ATR elements before moving them into the vented dry storage configurations at CPP-603. This chopping process reduced the element length to approximately 125.7 cm. The volume of a typical, cropped ATR ASNF element can be calculated by summing up the volumes of the 19 fuel plates (2,496 cm^3) and the two side plates (432 cm^3). This amounts to 2,928 cm^3 (Illum 1996). The surface area of a typical ATR element can be approximated by summing up the surface area of the 19 fuel plates and two side plates, which amounts to ~36,000 cm^2 (Hurt 2009).

3.3 ATR4 Buckets

The ATR4 bucket is a handling container for ATR ASNF elements that is currently used in some of INL's CPP-603 vented dry storage configurations. A sketch of the design is shown in Figure 3.

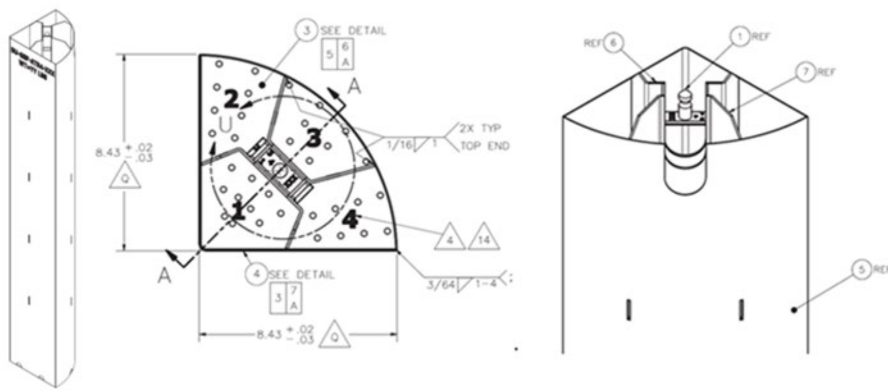

Figure 3. ATR4 bucket (adapted from [Orano 2019]).

Each bucket accommodates four ATR SNF elements. This study considered sealed dry storage configurations of eight ATR4 buckets, using two vertical levels, in a 10 × 18 DOE Standard Canister (for a total of 32 ATR ASNF elements) and of ten ATR4 buckets, using two vertical levels, in a 10 × 24 DOE Standard Canister (for a total of 40 ATR ASNF elements) (see Figure 4).

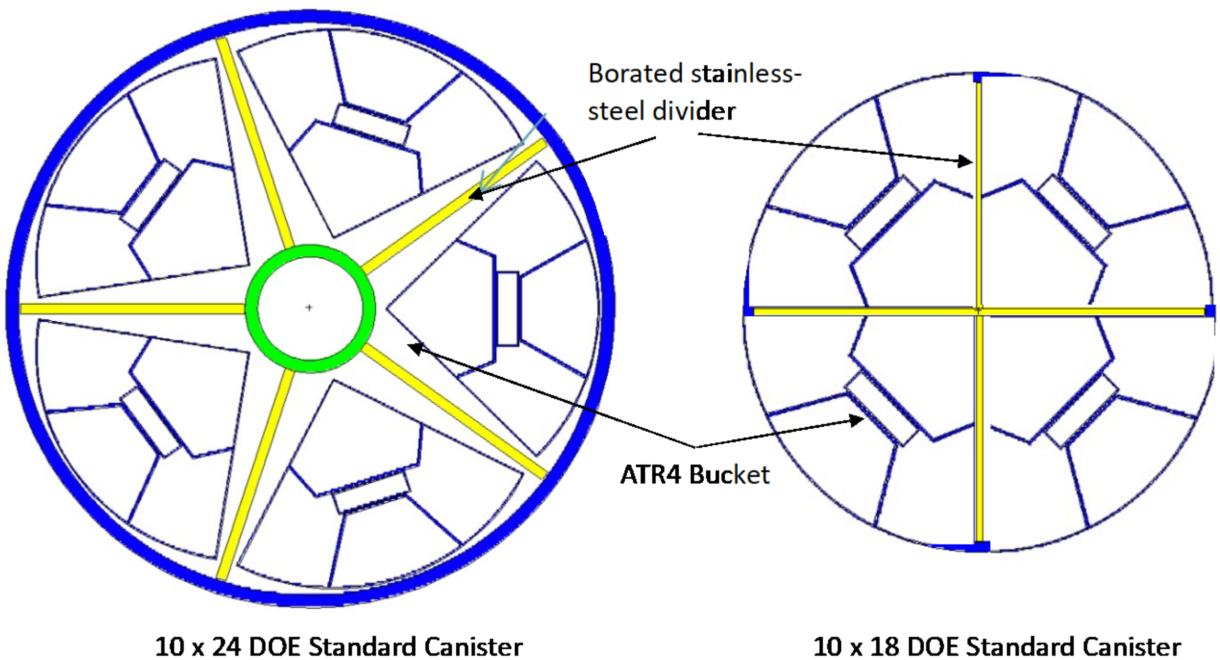

Figure 4. ATR4 bucket and basket structure within a 10 × 24 DOE Standard Canister (left) and 10 × 18 DOE Standard Canister (right) (adapted from [Orano 2019]).

Based on the geometrical data provided in Table 1, the total volume of the material that makes up a single ATR4 bucket is estimated as 4,125 cm^3. This estimate is conservative because it disregards the holes along the vertical sides of the ATR4 bucket (see Figure 3).

Table 1. Dimensions for the ATR4 bucket (Orano 2019).

Feature	Dimension
Base plate thickness	0.3048 cm
Outer wall thickness	0.1499 cm
Inner plate wall thickness	0.2667 cm
Center support thickness	0.3048 cm
Effective radius	21.4122 cm
Height to bottom of notch in inner plates	117.4496 cm
Height to top of center support plate	124.2822 cm
Overall height	128.5240 cm

3.4 Dividers and Spacer Disk

The considered DOE Standard Canister ASNF dry storage configurations include other components, such as two vertical levels of ATR4 bucket dividers ("baskets") made of borated stainless steel (see the green and yellow components in Figure 4). These baskets come with a wall thickness of ¼ in. and an estimated volume of 14,134 and 24,286 cm^3 for the 10 × 18 and 10 × 24 DOE Standard Canister configurations, respectively. Further, the considered configurations include a single 2-in.-thick circular spacer disk separating the two vertical ATR4 bucket and basket levels. The volumes of these spacer disks are estimated as 7,659 and 13,617 cm^3 for the 10 × 18 and 10 × 24 DOE Standard Canister, respectively. Table 2 provides a summary of the geometrical data provided above.

Table 2. Volumes and surface areas considered in the presented evaluations.

10 × 18 DOE Standard Canister	
Total canister cavity volume	382,974 cm^3
Volume of borated stainless steel basket	14,134 cm^3
Volume of eight ATR4 buckets	33,002 cm^3
Volume of one spacer disk	7,659 cm^3
Volume of 32 ATR ASNF elements	93,696 cm^3
DOE Standard Canister void volumes, in loaded condition, and 10% reduction	211,035 cm^3
Void volume as a fraction of total canister cavity volume	55.1%
Surface area of 32 ATR ASNF elements	1,152,000 cm^2
10 × 24 DOE Standard Canister	
Total canister cavity volume	660,416 cm^3
Volume of borated stainless steel basket	24,286 cm^3
Volume of ten ATR4 buckets	41,252 cm^3
Volume of one spacer disk	13,617 cm^3
Volume of 40 ATR ASNF elements	117,120 cm^3
DOE Standard Canister void volumes, in loaded condition, and 10% reduction	417,727 cm^3
Void volume as a fraction of total canister cavity volume	63.3%
Surface area of 40 ATR ASNF elements	1,440,000 cm^2

Note that the loaded DOE Standard Canister void volume is computed under a 10% reduction to consider remaining uncertainties in the configuration and component geometries. Further, note that the void volumes listed in Table 2 were estimated from computer-aided, three-dimensional models, and are ~2-5% smaller than the values used in the 2022 preliminary evaluations.

Additional details on the DOE Standard Canister design, loading configurations, internal components, and other system details can be found in various reports and sketches (see Morton 1999, Foster Wheeler Environmental Corporation 2002, and Orano 2019); however, the general operational loading procedures include placing the first vertical level of the two baskets into an open DOE Standard Canister shell (i.e., with a removed head assembly), moving four or five ATR4 buckets loaded with ATR ASNF elements into the basket compartments, placing the spacer disk, and continuing the loading process. After loading, the head assembly would be placed on top of the canister shell, and the canister would be welded shut (at the location of the "Backing Ring" in Figure 1). Eventually, the canister would be dried, evacuated, and backfilled with an inert helium gas.

3.5 Pressure and Flammability Evaluations—A Historical Perspective

3.5.1 Previously Established Design Limits

The *Preliminary Design Specification for DOE Standardized Spent Nuclear Fuel Canister* (Morton 1999) suggested a relatively low canister design pressure based off a maximum normal operating pressure of 150 kPag (22 psig) anticipated at a proposed geologic repository in 1998 (Abashian 1998). Subsequent drop tests confirmed that the pressure boundary integrity was well maintained for a canister pressurized to 50 psi (345 kPag) (Snow et al. 2000 and 2005). These canister pressure limits were not considered in the final repository license application in 2008, as the design requirements were transferred from the DOE Standard Canister to the repository waste package. Since then, finite element analysis modeling, combined with engineering calculations according to applicable codes and standards, has determined a permissible DOE Standard Canister pressurization that is upwards of 3,447 kPag (500 psig) at room temperature (Snow 2019). This range of modeling and testing campaigns indicate a highly robust DOE Standard Canister design capable of withstanding the most demanding, credible accident scenarios. However, it is important to recognize some degree of temperature impact on the DOE Standard Canister structural integrity, due to the expected softening of the stainless steel at elevated temperatures. This includes a limited reduction in permissible canister pressure at high temperatures, as demonstrated within this report.

Section 4.3.11 of the Waste Acceptance System Requirements Document (U.S. DOE 2008) excludes flammable DOE Standard Canisters from disposition in a Civilian Radioactive Waste Management System (CRWMS) (i.e., the deep geological repository Yucca Mountain in Nevada):

> *Factors such as pyrophoricity, explosivity, combustibility, chemical reactivity, gas generation, thermal effects, particulate concentrations, internal corrosion of the canister and the contained material, and any other relevant factors, shall be prevented or mitigated prior to acceptance into the CRWMS such that the canister and its contents shall not cause a fire or explosion at the receiving facility during normal handling operations and following a canister drop.*

To meet these requirements, established H_2 and O_2 concentration limits (i.e., lower flammability limits [LFLs]) can be credited in DOE Standard Canister flammability evaluations. For instance, generally recognized minimum H_2 concentrations in air or a pure oxygen atmosphere to reach flammability are 4 vol.% (Zabetakis 1965). Previous work on the Multi-Canister Overpack, a realized dry storage canister concept for DOE SNF at the Hanford site, led to the engineering demonstration that a gas mix with less than 4 vol.% O_2 can be considered non-flammable (Bader 2010), which aligns with findings of studies on the limiting oxygen concentration and flammability limits in H_2 conducted by Zlochower and Green (Zlochower and Green 2009). The U.S. Nuclear Regulatory Commission also recognizes oxygen limits as a method of flammability control, suggesting a 5 vol.% oxygen limit for waste shipment packages or portions of waste shipment packages with a hydrogen concentration greater than 5% (U.S. NRC 1984). Pertaining to the present DOE Standard Canister flammability evaluations, it is assumed that flammability is only achievable if gaseous concentrations of H_2 and O_2 within the internal canister atmosphere reach or exceed LFLs of 5 or 4 vol.%, respectively. Drying of SNF storage canisters is a common approach to limit H_2 generation. Backfilling these canisters with an inert gas, such as helium, is a common approach to control the O_2 concentration. Both methods are anticipated to be included in ASNF DOE Standard Canisters conditioning processes.

3.5.2 Previously Conducted Pressure and Flammability Evaluations

In 2007, INL conducted a material interaction evaluation to determine the pressurization for ATR ASNF packaged into three vertically stacked Type 1a baskets within a sealed 15 × 18 DOE Standard Canister, during dry storage periods of 50 years (Hurt 2009). Each Type 1a basket contained 10 ATR ASNF elements (see Figure 5). This evaluation was made under the assumption that chemisorbed water was bound within a 34-µm-thick monohydrate (boehmite [$Al_2O_3 \cdot H_2O$]) aluminum oxide layer adhered to the SNF surface area. The thickness of this layer was based on the assumption of 9% ATR cladding thinning during in-reactor operation (Illum 1996). Further, it was assumed that all residual water would be broken down and all available H_2 would be released, the computed upper limit canister pressurization was limited to 334 psi (2,372 kPa) at 315°C. Furthermore, Hurt's computation assumed that all available O_2

would remain bound or would become bound to the ASNF surface, and thus, would not contribute to the canister pressurization.

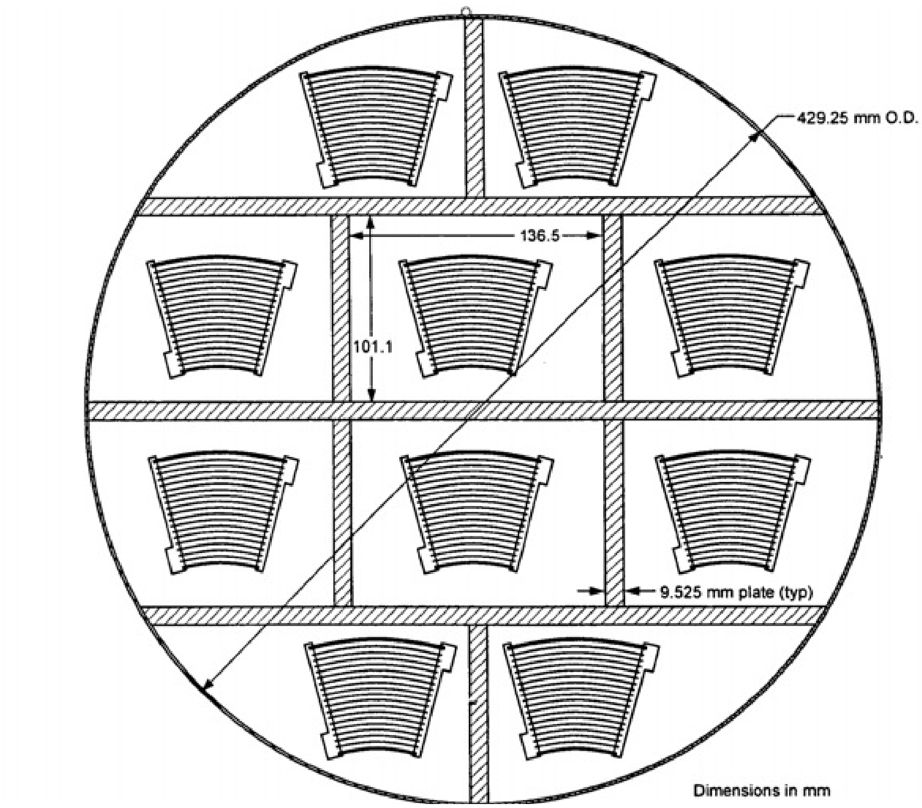

Figure 5. Type 1a basket containing ATR SNF.

Since 2017, DOE EM has been sponsoring activities executed at INL with collaborators throughout the DOE complex to address issues related to the management, storage, transportation, and disposal of DOE-owned SNF through technology development (TD) (Jarrell and Eidelpes 2022 and Eidelpes et al. 2023). Significant work has been completed to address concerns related to storing ASNF over an extended period of time (>50 years), which included a range of modeling and simulation (M&S) activities (Abboud 2021). Within these activities, computational fluid dynamics (CFD) models were developed to feed a complex chemical model—representing the chemical processes ongoing in an ASNF dry storage canister—with thermal data. Unlike the simple hand calculations presented in this report, this chemical model considered 115 gas phase reactions to analyze the generation of a variety of chemical species and pressure build up (among other parameters of interest). One of the analyzed configurations is a 15 × 18 DOE Standard Canister, loaded with 30 ATR ASNF elements within three Type 1a baskets. A range of assumptions were made during these efforts, such as H_2 generation rates (i.e., G-values) and oxide layer thicknesses (up to 15 μm), based on a broad range of accompanying ASNF examination activities and radiolytic gas generation experiments (e.g., Parker-Quaife et al. 2020 and Conrad et al. 2022). These models indicate a pressure buildup of up to ~2.56 atm (~259 kPa) and the generation of an H_2 concentration >15%, respectively, during 50 years of dry storage. A negligible generation of oxygen species was reported. Further, an insignificant increase in pressure, and in H_2 and O_2 concentrations was predicted for longer durations (up to 200 years) (Abboud 2022).

At this point in time, these DOE EM SNF TD M&S activities represented the most sophisticated work to determine the internal conditions of ASNF dry storage canisters utilizing Type 1a basket configurations. However, the activities were not representative of a maximum loading configurations proposed in a 2019 report on geometrical fit and criticality safety for ASNF in a DOE Standard Canister (Orano 2019). These configurations enable loading 32 ATR ASNF elements into a 10 × 18 DOE Standard Canister[b] or up to 40 ATR ASNF elements into a 10 × 24 DOE Standard Canister (see Figure 4). Instead of loading individual ATR ASNF elements into a DOE Standard Canister basket (such as the previously considered Type 1a basket), these new configurations utilize so-called ATR4 buckets, each carrying four individual ATR ASNF elements. These buckets are currently used in vented ATR dry storage configurations at INL's CPP-603 facility and facilitate handling four ATR elements at a time. As described above, the ATR ASNF element handling features were cut off when transferring them to CPP-603 vented dry storage, thus making it difficult to handle single elements.

These new, dense storage configurations required an update in the evaluations that had been completed up to this point. Thus, corresponding, preliminary pressure and flammability evaluations were initiated in 2022. The utilized approach was based on Hurt's 2009 hand calculations, and similar, highly conservative assumptions were made, such as a full radiolytic breakdown of the chemisorbed water in the canister, a oxide layer thickness of 34 µm, and a maximum gas temperature of up to 343°C. To study the impact of oxide layer type on canister pressurization and flammability, these preliminary evaluations considered trihydrate and monohydrate oxide layers. Note that 343°C represents the maximum primary service temperature for a DOE Standard Canister after emplacement within another enclosed container (Morton 1999). Although the findings of these preliminary evaluations indicate that the pressure could exceed the structural integrity limit of ~500 psig (3,447 kPa) established by Snow (Snow 2019), this exceedance is limited to selected cases (i.e., to cases that include 10 × 18 DOE Standard Canister configurations, trihydrate oxide layers and temperatures above 200°C). The computed H_2 concentration exceeded the LFL of 5% in all of the considered scenarios. However, these preliminary findings need to be interpreted within the context of the conservative assumptions made, such as the presence of trihydrate and the full radiolytic breakdown of water. Further, the absence of O_2 would prevent the creation of a flammable atmosphere in the canister.

To confirm the accuracy and conservatism of these 2022 findings, additional M&S efforts were completed in early 2023 (Abboud and Morco 2023). 10 × 18 and 10 × 24 DOE Standard Canister loaded with 32 and 40 ATR ASNF elements within ATR4 buckets were simulated, and the previously developed chemical model was modified to achieve a full release of available H_2 from an assumed boehmite layer with a thickness of up to 34 µm under dried and undried conditions (Under undried conditions, chemisorbed and physiosorbed water is released from the surface, such that water vapor radiolysis could occur. However, chemical equilibrium of the modeled reactions does not show the full breakdown of water vapor into O_2 and H_2. Under high temperature conditions, general corrosion of aluminum occurs slowly converting water into aluminum oxide and hydrogen). The results of these M&S efforts aligned with the preliminary 2022 findings, that is, a canister pressurization above 500 psig (3,447 kPa) for selected 10 × 18 configurations under consideration of a 34 µm thick undried conditions at temperatures above 200°C, an H_2 concentration above the LFL of 5%, and the absence of significant concentrations of any oxygen species.

This report builds on the 2022 preliminary evaluations and will be the document of record for these calculations as additional information has been identified. For example, the credible range of the oxide layer thickness adherent to the ASNF (d'Entremont and Sindelar 2023) has been updated. Further, the absence of oxygen species—one of the key species needed to generate a flammable atmosphere—in helium-backfilled ASNF dry storage configurations was confirmed (Conrad and Horne 2023). Furthermore, CFD models of anticipated DOE Standard Canister dry storage configurations provided improved estimates for realistic upper limit canister atmosphere temperatures (Murphy-Sweet 2022). Additionally, steady-state structural evaluations of the canister pressure structural limit at elevated

[b]Note that, due to the accumulation of manufacturing tolerances of individual components, the feasibility of this configuration remains uncertain.

temperatures are provided, enabling the comparison of these refined pressure estimates with pressure limits computed according to the applicable codes (i.e., the ASME BPVC Section III – Rules for Construction of Nuclear Facility Components – Division 3 – Containment Systems & Transport Packagings for Spent Nuclear Fuel & High Level Radioactive Waste). These new insights, combined with refined estimates of geometrical parameters, such as DOE Standard Canister void volume, allow for conducting more realistic bounding pressure and flammability evaluations, which are presented herein.

4. METHODOLOGY

4.1 Assumptions

The following assumptions are made within the scope of the presented evaluations of the bounding pressure and flammability evaluations:

1. Assumption: All chemisorbed, physisorbed, and free water is broken down in a radiolytic gas generation process.
   Basis: This is a highly conservative key-assumption that forms the bounding character of the presented bounding pressure and flammability evaluations.[c]
2. Assumption: Table 3 summarizes the assumptions made on the chemical species created in the radiolytic gas generation process.

   Basis: Recent studies of available data on O_2 yield from corroded aluminum alloys confirm H_2 generation (e.g., Parker-Quaife 2020) and the absence of oxygen species (Conrad and Horne 2023). Data from recently completed chemical M&S align with these findings (e.g., Abboud 2021). This is not necessarily the case in the radiolytic breakdown process of free water, which could lead to the release of H_2 and O_2. These species could theoretically form gaseous oxyhydrogen (2:1). Note that the consideration of oxyhydrogen generation from free water is more conservative than the assumption of a reaction of oxygen species with the ASNF surface made by Hurt (2007) as well as in the 2022 preliminary evaluations. However, recently completed ASNF drying experiments suggest the availability of drying processes that are highly effective in removing free water (Perry et al. 2021), and the impact of this additional conservatism on the results of the presented evaluations will be limited to small quantities of residual steam due to imperfect canister evacuation and a hypothetically considered quantity of residual free water in sensitivity studies. Further, although Perry et al.'s findings do not draw definitive conclusion on the effectiveness of the tested drying procedures in completely removing physisorbed water, for the purpose of the present evaluations it is assumed that appropriate processes and equipment are used to ensure removal of such.

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[c]Note that high cladding temperatures during storage could be sufficient for releasing water vapor from corrosion layers (Perry et al. 2021), autonomous of a radiolytic gas generation process. However, recently completed CFD simulations (Murphy-Sweet 2022) indicate that such temperatures (>220°C) would not be reached in the presently considered ASNF dry storage configurations. Further, high-temperature drying exceeding 220°C could trigger such a release during canister conditioning (i.e., initiating a phase transition of present trihydrate oxide layer types to monohydrates) (Perry et al. 2021), forestalling this process during storage.

Table 3. Hydrogen and oxygen species created in the radiolytic breakdown process.

Source of H_2O	**Chemical Species**	**Note**
Chemisorbed	H_2	Oxygen remains trapped in oxide layers.
Physisorbed	H_2	Oxygen remains trapped in oxide layers. This assumption applies to the hypothetically evaluated scenarios of physisorbed, residual water within the canister. No physisorbed water is assumed to remain within the considered ASNF dry storage configurations after drying.
Free (including steam)	H_2, O_2	Oxyhydrogen (2:1) is created. This is a hypothetical scenario as the simulations of the chemical processes do not point to the formation of gaseous O_2. Further, no significant amount of free water is expected to remain within the considered ASNF dry storage configurations after drying.

3. Assumption: A DOE Standard Canister loaded with ATR SNF is the limiting case for the presented evaluations. The two considered dry storage configurations included two vertical levels of ATR SNF on top of each other. The first configuration includes a 10 × 18 DOE Standard Canister loaded with four ATR4 buckets in each of the two vertical levels, providing space for a total of 32 ATR ASNF elements within the canister. The total ASNF surface area of this configuration is 1,152,000 cm^2. The second configuration includes a 10 × 24 DOE Standard Canister loaded with five ATR4 buckets in each of the two vertical levels, providing space for a total of 40 ATR ASNF elements within the canister. The total ASNF surface area of this configuration is 1,440,000 cm^2.

   Basis: This configuration selection was based on comparisons of ATR ASNF with other DOE-managed ASNF types. Indicating relatively thick corrosion layers adherent to its large surface area, ATR ASNF could retain large quantities of chemisorbed water. Further, this ASNF type has a relatively high decay heat, which could promote radiolysis and pressure generation. Furthermore, the considered ATR ASNF DOE Standard Canister configurations have a high ratio of ASNF surface to canister void volume and thus should present a bounding case for canister pressurization and H_2 concentration (Abboud 2021). Furthermore, these configurations were modeled in a criticality and geometrical fit analysis for ATR SNF in a DOE Standard Canister [Orano 2019]. Note that the configurations in the present evaluations are different from the configuration previously evaluated using Type 1a baskets in a 15 × 18 DOE Standard Canister (Hurt 2007).

4. Assumption: The expected, average oxide layer thickness on the ATR ASNF is limited to 25 µm.

   Basis: This is lower than the previously estimated oxide layer thickness of 34 µm suggested by Hurt (2009). The reduction from 34 to 25 µm is based on ASNF examination activities and reviews of reported empirical observations: A recently completed, comprehensive review of the available data of oxide layer thicknesses adherent to a range of ASNF types indicate an average thickness that could range from 12 to 25 µm (d'Entremont and Sindelar 2023). Note that a level of uncertainty remains in this assumption, given that localized oxide layer thickness values of up to 80 µm were reported. Thus, it is recommended to reevaluate the safety of the considered ASNF dry storage configurations if future ASNF examination activities indicate the presence of higher average oxide layer thickness values.

5. Assumption: The considered oxide layer is a trihydrate layer with a density of 2.43 g/cm^3 and a water content of 34.6 wt.%.

   Basis: The oxide layer types found on ASNF often appear in mixed layers containing at least two types, including gibbsite, bayerite ($Al_2O_3 \cdot 3H_2O$), and boehmite ($Al_2O_3 \cdot H_2O$) (Olson et al. 2018 and 2019). Although high temperature drying above 220°C will likely lead to a phase transition from monohydrates to trihydrates, which can be associated with the additional removal of chemisorbed water (Perry et al. 2021), an ASNF drying procedure has yet to be defined. Thus, an oxide layer comprised, at least partially, of trihydrate, cannot be excluded.

The *Engineering-Scale Drying of Aluminum-Clad Spent Nuclear Fuel* report suggests a pure gibbsite or bayerite (i.e., trihydrate) layer density of 2.43 g/cm^3 (Perry et al. 2021). This is lower than the density of a pure boehmite (i.e., monohydrate) layer (3.01 g/cm^3) (Hurt 2009). However, Perry et al. (2021) suggested a trihydrate water content of 34.6 wt.%, which eventually yields a larger mass of chemisorbed water per volume bound in this trihydrate, compared to the mass of chemisorbed water in monohydrate (which has an assumed water content of 15 wt.% [Hurt 2007]). This larger water mass makes the assumption of a trihydrate layer conservative pertaining its potential of H_2 yield.

6. Assumption: The drying process removes all free and physisorbed water other than residual steam due to imperfect canister evacuation from the DOE Standard Canister cavity and atmosphere before backfilling the canister with helium.

   Basis: Recently completed ASNF drying experiments point to effective removal of free water during commonly used and readily available SNF drying procedures (Perry et al. 2021). Although Perry et al.'s findings do not draw definitive conclusion on the effectiveness of the tested drying procedures in completely removing physisorbed water, for the purpose of the present evaluations it is assumed that appropriate processes and equipment are used to ensure removal of such. This aligns with the assumptions made by Hurt (2009).

   The two considered drying procedures to condition the considered ATR ASNF DOE Standard Canister configurations include vacuum drying and forced helium dehydration. Evacuating the canister during vacuum drying or after forced helium dehydration (prior to helium backfilling) will drastically lower the internal canister pressure. The targeted vacuum quality is 3 torr at 25°C, controlling the quantity of remaining gas, which is close to the 3 torr at 45°C bounding limit established by the Hanford site for drying of the Multi-Canister Overpacks (Hurt 2009). The residual gas could be steam subject to the (hypothetical) radiolytic generation of oxyhydrogen or other chemical species. Realistically, however, the impact of this radiolytic gas generation process should remain insignificant on both pressure and flammability, if the canister is evacuated properly. Additional studies demonstrating the importance of proper canister evacuation before helium backfilling can be found in APPENDIX A of this report.

7. Assumption: An average gas temperature and DOE Standard Canister shell temperature of 220°C is the maximum credible temperature during normal conditions of storage.[d]

   Basis: Recently completed CFD simulations point to a peak gas temperature of 198.1°C under normal conditions of the envisioned DOE Standard Canister dry storage configurations (Murphy-Sweet 2022). These simulations included nine DOE Standard Canisters loaded within a stainless steel overcanister within a concrete overpack. The overcanister is backfilled with argon. Further, these studies indicate a lower canister shell material temperature (171.1°C), thus making the assumption of a DOE Standard Canister shell temperature equal to the average gas temperature conservative. Furthermore, within the present evaluations, a safety margin of ~10% covers for uncertainties in the final storage configurations, limiting the considered gas temperature to 220°C or less.

8. Assumption: The considered DOE Standard Canister void volumes (in loaded condition) as fractions of the (empty) canister cavity volumes are summarized in Table 4.

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[d]Note that this temperature is below the DOE Standard Canister Primary Service Temperature of 343.3°C after placement within another enclosed container, as defined in Morton (1999). The selection of 220°C was made for bounding pressure evaluations purposes for the considered dry storage configurations only, and is only meaningful within the context of such. The authors do not challenge the preliminary design specifications of the DOE Standard Canister. Higher temperatures remain possible for different dry storage or disposal configurations. These higher temperatures would allow for higher pressures within the canister.

Basis: These volumes are computed based on recently completed three-dimensional DOE Standard Canister models and estimations. Further, a safety margin of 10% of the absolute value reduces the void volume and accounts for uncertainties in the volume of smaller canister-internal components. This reduction conservatively increases the pressure resulting from the gaseous species within the canister.

Table 4. DOE Standard Canister void volumes, in loaded condition and after reduction by 10%.

DOE Standard Canister Type	Loaded DOE Standard Canister Void Volume [% of Empty Canister Cavity Volume]
10 × 18	55.1%
10 × 24	63.3%

9. Assumption: The DOE Standard Canister corrosion is limited to 10% of the canister shell wall thickness, and the corrosion layer is located inside the canister shell and head. Further, consideration of canister corrosion is limited to permissible canister pressure evaluations but is disregarded in the computations of the canister pressure.

   Basis: No significant corrosion of the DOE Standard Canister itself is expected due to the use of stainless steel, an inert canister backfill atmosphere, and limited generation of corrosive species, such as nitric acid (Abboud 2021). Further, no significant external canister corrosion is expected due to the use of stainless steel in the DOE Standard Canister design (and possibly, the use of an inert overcanister backfill gas, such as argon, when storing multiple DOE Standard Canisters within a welded overcanister). However, a corrosion safety margin is utilized to cover for uncertainties in the final DOE Standard Canister dry storage configurations, by modifying the canister geometry when computing the permissible canister pressure. The selected margin is equal to 10% of the nominal canister shell wall thickness after consideration of manufacturing tolerances. Internal canister corrosion generally leads to lower permissible canister pressures than external corrosion.

10. Assumption: The DOE Standard Canister is backfilled with helium with a pressure of 27.6 kPag (4 psig) at 21°C.

    Basis: The design specification for the DOE Standard Canister specifies a helium backfill pressure of 13.8–27.6 kPag (2-4 psig) (Morton 1999). This is close to the ~5 psig (~35 kPag) value suggested by Hurt (2009). Choosing 27.6 kPag increases the initial gas quantity in the DOE Standard Canister, thus increasing the maximum potential pressure. Choosing the lower limit of 13.8 kPag (2 psig) would decrease the amount of helium in the canister atmosphere and increase the potentially achievable H_2 and O_2 concentrations; however, these concentrations are expected to remain insignificant. Note that, due to specification of the helium backfill pressure at gauge, the quantity of backfill gas within the DOE Standard Canister is impacted by the achieved vacuum quality prior to backfilling and the atmospheric pressure of the DOE Standard Canister environment during backfilling.

11. Assumption: The atmospheric pressure of the DOE Standard Canister loading and storage location environment is at least 0.5 atm (50.7 kPa).

    Basis: Information on the minimum atmospheric pressure of the DOE Standard Canister environment is needed to evaluate canister integrity by computing the difference between the internal and external pressure. The considered DOE Standard Canister configurations will be loaded at INL's CPP-603 facility, which is ~1,500 m above sea level. A maximum altitude of the final storage location of 3,000 m was assumed. The considered possible lowest atmospheric pressure at sea level is 87 kPa (0.85 atm), and an adjustment factor of 1.2 kPa (0.01184 atm) for every 100 meters of altitude was used to adjust this minimum pressure for the final storage altitude (i.e., 0.5 atm).

12. Assumption: There are no credible mechanisms for moisture to be added to a sealed DOE Standard Canister.

Basis: Breaching a sealed DOE Standard Canister is a hypothetical, non-mechanistic event (Carlsen 2004). Drop tests and available results of structural evaluations indicate a highly robust DOE Standard Canister design is capable of withstanding the most demanding, credible accident scenarios (Snow et al. 2005 and Snow 2019). Without a breach, moisture cannot enter the DOE Standard Canister.

13. Assumption: Pertaining to the present DOE Standard Canister flammability evaluations, it is assumed that flammability is only achievable if gaseous concentrations of H_2 and O_2 within the internal canister atmosphere reach or exceed LFLs of 5 or 4 vol.%, respectively.

    Basis: Generally recognized minimum H_2 concentrations in air or a pure oxygen atmosphere to reach flammability are 4 vol.% (Zabetakis 1965). Previous work on the Multi-Canister Overpack, a realized dry storage canister concept for DOE SNF at the Hanford site, led to the engineering demonstration that a gas mix with less than 4 vol.% O_2 can be considered non-flammable (Bader 2010), which aligns with findings of studies on the limiting oxygen concentration and flammability limits in H_2 conducted by Zlochower and Green (Zlochower and Green 2009). The U.S. Nuclear Regulatory Commission also recognizes oxygen limits as a method of flammability control, suggesting a 5 vol.% oxygen limit for waste shipment packages or portions of waste shipment packages with a hydrogen concentration greater than 5% (U.S. NRC 1984).

These assumptions were used to evaluate the bounding conditions within the considered ATR ASNF DOE Standard Canister configurations. However, to study the sensitivity of canister pressure or flammability, some of the relevant parameters and assumptions were modified to include hypothetical values in exemplary demonstrations of the utilized methodology. These modifications are not necessarily realistic and thus irrelevant to evaluating the bounding conditions under the currently expected DOE Standard Canister configurations.

4.2 The Standard Canister Pressure Estimator

The presented analyses were completed utilizing a computation tool, the Standard Canister Pressure Estimator (SCPE). This tool was developed using Python 3, allowing for rapid estimation and documentation of upper bound pressure values for specific DOE Standard Canister ASNF dry storage configurations. This supports the identification of pressure- or flammability-relevant parameters, which is one of the main objectives of the presented work. One of the key assumptions of SCPE is a full radiolytic breakdown of the residual water in the considered configuration, which is consistent with the assumptions in this report. Note that SCPE is a conceptual software, a documentation on the functionalities of the tool has yet to be developed, and a detailed description of this tool is outside the scope of the present report; however, a snapshot of the SCPE graphical user interface is shown in Figure 6, and SCPE data output files documenting the conducted computations are in APPENDIX B.

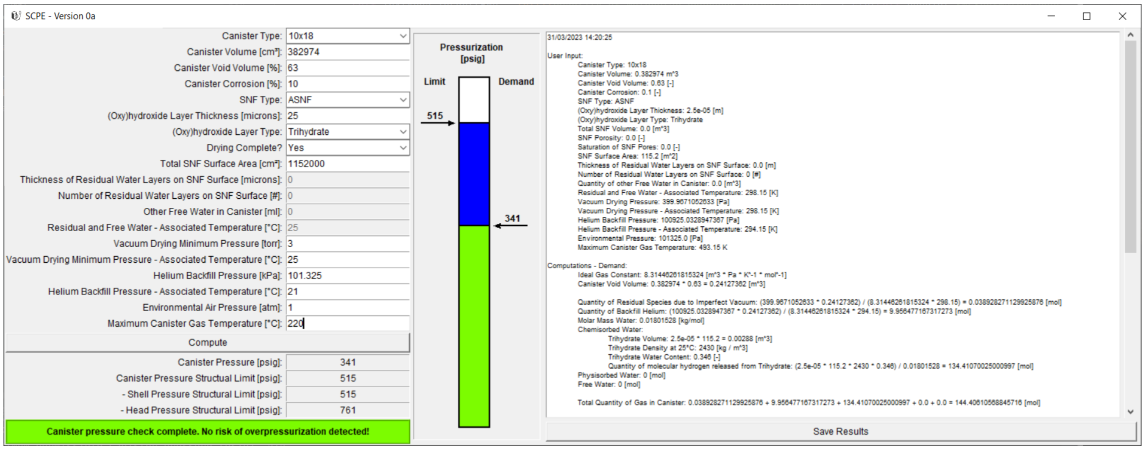

Figure 6. SCPE graphical user interface.

4.3 Computations

4.3.1 Maximum Pressure

Equation 1 quantifies the amount of H_2 ($n_{hydrogen}$, in moles) released due to the full radiolytic breakdown of chemisorbed water bound in the oxide layers on the ASNF:

$$n_{hydrogen} = \frac{\rho_{oxide} \times t_{oxide} \times A \times WC}{MR_{water}} \tag{1}$$

where ρ_{oxide} is the density of the oxide layer, t_{oxide} is the oxide layer thickness, A is the surface area of the ASNF, WC is the water content, and MR_{water} is the molar mass of water.

Equation 2 computes the quantity of H_2 ($n_{hydrogen}$, in moles) released due to the full radiolytic breakdown of physisorbed water within the canister; although, it assumed that all physisorbed water is removed during ASNF dry storage conditioning:

$$n_{hydrogen} = \frac{\rho_{water} \times t_{water} \times A}{MR_{water}} \tag{2}$$

where ρ_{water} is the density of the water layer at the specified temperature (computed according to the equation developed by Kell [1975]), t_{water} is the water layer thickness, A is the surface area of the ASNF, and MR_{water} is the molar mass of water.

The Ideal Gas Law (Equation 3) computes the quantity of oxyhydrogen (2:1) ($n_{oxyhydrogen}$, in moles) potentially released due to the full radiolytic breakdown of residual water steam within the canister:

$$n_{oxyhydrogen} = \frac{p_{vacuum} \times V}{R \times T} \times 1.5 \tag{3}$$

where p_{vacuum} is the achieved vacuum quality, V is the DOE Standard Canister void volume (in loaded condition), R is the ideal gas constant, and T is the temperature associated with the achieved vacuum quality. The factor of 1.5 accounts for the quantity of pressure generating molecular oxygen (O_2) in the 2:1 (H_2:O_2) mix in the oxyhydrogen.

Equation 4 can be used to compute the quantity of oxyhydrogen (2:1) ($n_{oxyhydrogen}$, in moles) potentially released due to full radiolytic breakdown of free water within the canister; although, it assumed that all free water is removed during ASNF dry storage conditioning:

$$n_{oxyhydrogen} = \frac{\rho_{water} \times V_{water}}{MR_{water}} \times 1.5 \tag{4}$$

where ρ_{water} is the density of the free water at the specified temperature (computed according to the equation developed by Kell [1975]), V_{water} is the volumetric amount of free water in the canister, and MR_{water} is the molar mass of water. The factor of 1.5 accounts for the pressure generating molecular oxygen (O_2) in the 2:1 (H_2:O_2) mix in the oxyhydrogen.

The Ideal Gas Law (Equation 5) computes the quantity of helium (n_{helium}, in moles) introduced into the canister during backfilling:

$$n_{helium} = \frac{(p_{backfill} - p_{vacuum}) \times V}{R \times T} \tag{5}$$

where $p_{backfill}$ is the absolute backfill pressure at the specified temperature computed under a specified atmospheric pressure (assuming an identical temperature), $p_{vacuum}$is the achieved vacuum quality adjusted to the temperature during backfilling, V is the DOE Standard Canister void volume (in loaded condition), R is the ideal gas constant, and T is the temperature associated with the backfill pressure.

Eventually, the Ideal Gas Law (Equation 6) is used to compute the canister pressurization.

$$p = \frac{\sum n \times R \times T}{V} \tag{6}$$

where $\sum n$ is the summation of the quantities of the individual gaseous species within the canister computed with Equations (1) to (5), p is the absolute canister pressure at the specified temperature T under the DOE Standard Canister void volume V (in loaded condition), and R is the ideal gas constant.

4.3.2 Permissible Department of Energy Standard Canister Pressure

The permissible DOE Standard Canister pressure is computed according to ASME BPVC.III.3-2021 and loosely follows the methodology outlined in Snow's hand calculations (Snow 2019). It is dependent on the selected canister geometry, material type, and temperature. Note that, unlike Snow, the present evaluations assume normal operating conditions (i.e., do not consider canister impact scenarios). Further, one of the pressure limit controlling variables in these computations is the material temperature (which is assumed to be equal to the specified canister atmosphere temperature, see Assumption 7), because it affects the canister material strength. The DOE Standard Canister is made of 316L stainless steel, and the design stress intensity of this material decreases with increasing temperature (see ASME BPVC.II.D.C-2021 Table 2A, Row 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603). Note that ECAR-4632 computed a permissible canister pressure upwards of 500 psig (3,447 kPa) at room temperature (Snow 2019), and no significant impact of the considered material temperature is expected. However, considering the effects of an elevated material temperature on the permissible canister pressure allows for a more consistent comparison with the pressure demand at temperature. Further, note that the code limits the acceptable material temperature to ~426°C (800°F) (see ASME BPVC.III.3-2021 WB-3112.2).

Table 5 summarizes the geometrical parameters used in this report, assuming corrosion equal to 10% of the nominal canister shell wall and a 12.5% canister shell wall thickness tolerance (according to ASME BPVC.II.A-2021 SA-312/SA-312M Table 3).

Table 5. DOE Standard Canister geometrical parameters used to compute the permissible pressure.

10 × 18 DOE Standard Canister	
Internal corrosion layer thickness	0.95 mm
Canister shell wall thickness, corroded, 12.5% tolerance	7.5 mm
Canister shell inner radius, corroded	221.1 mm
Canister head wall thickness, corroded	14.9 mm
Canister head sphere radius, corroded	454.98 mm
Canister head diameter at shell interface location, corroded	433.7 mm
Canister head knuckle radius, corroded	28.7 mm
10 × 24 DOE Standard Canister	
Internal corrosion layer thickness	1.27 mm
Canister shell wall thickness, corroded, 12.5% tolerance	10 mm
Canister shell inner radius, corroded	294.8 mm
Canister head wall thickness, corroded	19.4 mm
Canister head sphere radius, corroded	607.7 mm
Canister head diameter at shell interface location, corroded	578.8 mm
Canister head knuckle radius, corroded	38.6 mm

ASME BPVC.III.3-2021 suggests computing the permissible canister pressure as the minimum of the permissible canister shell pressure and the permissible canister head pressure. The permissible canister shell pressure is calculated according to WC-3224.3. The permissible canister head pressure is computed according to WC-3224.8. Ultimately, the canister pressure computed according to Equation 6 at gauge is compared with the permissible canister pressure computed according to ASME BPVC.III.3-2021.

4.3.3 Flammability Evaluations

The flammability of the canister atmosphere is evaluated by computing the H_2 and O_2 concentrations in the atmosphere and comparing it to the 5% and 4% LFLs, respectively. Both concentrations need to exceed their respective limit. Equations (1) to (4) are used to compute the amount of generated H_2, which is equal to the sum of the results of Equations (1) and (2) and 2/3 of the sum of the results of Equations (3) and (4) (i.e., one mole H_2 per mole chemisorbed water, physisorbed water, free water, or steam). Equations (3) and (4) are used to compute the amount of generated O_2, which is equal to 1/3 of the sum of the results of these individually evaluated equations (i.e., one mole O_2 per two moles of free water or steam). Then, the H_2 and O_2 concentrations are computed by dividing these amounts by the total amount of gaseous species within the canister. Eventually, the flammability of the canister atmosphere is evaluated by comparing the molar concentration of H_2 and O_2 in the canister with the LFL of 5% and 4%, respectively, as established in Assumption 13.

Note that the assumption of O_2 release from free water and steam is a conservative assumption, since no O_2 generation in systems containing corroded aluminum under gamma radiation has been detected (Conrad and Horne 2023). Further, no free water (other than limited amounts of steam) is expected to remain in a dry canister. Furthermore, a canister breach that could lead to water intrusion is not considered a credible scenario.

5. RESULTS

Table 6 summarizes the significant parameters in the bounding pressure and flammability evaluations. Case 1 represents the 10 × 18 DOE Standard Canister configuration, and Case 2 represents the 10 × 24 DOE Standard Canister configuration.

Table 6. Considered parameters in the bounding cases.

Case	**1**	**2**
Canister type	10 × 18	10 × 24
Number of ATR ASNF elements	32	40
Free void volume	55.1%	63.3%
Total ASNF surface area	1,152,000 cm^2	1,440,000 cm^2
Canister corrosion	10%	10%
Oxide layer type	Trihydrate	Trihydrate
Oxide layer thickness	25 µm	25 µm
Oxide layer density	2.43 g/cm^3	2.43 g/cm^3
Oxide layer water content	34.6%	34.6%
Amount of physisorbed water	None	None
Amount of free water	None	None
Vacuum quality	3 torr at 25°C	3 torr at 25°C
Helium backfill pressure	27.6 kPa at 21°C	27.6 kPa at 21°C
Atmospheric pressure environment	0.5 atm at 21°C	0.5 atm at 21°C
Gas and canister material temperature	220°C	220°C

Table 7 summarizes the results of the pressure and flammability evaluations. The associated SCPE output files can be found in APPENDIX B.

Table 7. Results of bounding pressure and flammability evaluations.

Case	**1**	**2**
Bounding pressure	391 psig (2,696 kPag)	251 psig (1,729 kPag)
Permissible pressure[e]	515 psig (3,553 kPag)	515 psig (3,553 kPag)
Structural integrity concern?	No	No
Total quantity of gaseous species	141.18 mol	181.42 mol
H_2 quantity and concentration	0.05 * 2 / 3 + 134.41 = 134.44 mol (95.23%)	0.10 * 2 / 3 + 168.01 = 168.08 mol (92.64%)
O_2 quantity and concentration	0.05 * 1 / 3 = 0.02 mol (0.01%)	0.10 * 1 / 3 = 0.03 mol (0.02%)
Flammability concern?	No	No

5.1 Sensity Studies

Sensitivity studies were conducted to identify the pressure and flammability controlling parameters. Table 8 summarizes a list of parameters that were modified in these studies, including a qualitative assessment of the associated levels of uncertainty in the parameter values (based on the available research summarized in the sections above and the judgment of the authors) and the parameter value modification needed to reach critical pressure values or raise flammability concerns. Eventually, the “Level of Control” column—developed under consideration of parameter uncertainties and the magnitudes of base value modification needed to cause a safety issue—provides a basis for the authors interpretation of the potential of the parameter to impact the canister safety.

[e]Note that the permissible pressure of the 10 × 18 and 10 × 24 DOE Standard Canister versions is identical, despite their different geometries. This is due to the similar proportions of the geometrical parameters (such as wall thickness to radius) used in the design of both versions.

Table 8. Findings of the sensitivity studies.

Parameter	Qualitative Assessment of Parameter Uncertainty	Modification of Base Value Needed to Raise a Safety Concern	Level of Control
Free void volume	Medium	Case 1: -25% (Overpressurization)	Medium
Total ASNF surface area	Low	Case 1: + 34% (Overpressurization)	Low
Canister corrosion	Medium	Case 1: +216% (Overpressurization)	Low
Oxide layer type	Large	Worst case was considered	Low
Oxide layer thickness	Medium	Case 1: +33% (Overpressurization)	Medium
Oxide layer density	Medium	Case 1: +33% (Overpressurization)	Medium
Oxide layer water content	Medium	Case 1: +33% (Overpressurization)	Medium
Amount of physisorbed water	Low	Case 1: Adding one physisorbed water layer of 7 µm to entire SNF surface area (Overpressurization)	Low
Amount of free water	Low	Case 1: Adding 235 ml of free water (Flammability)	Low
Vacuum quality	Low	No safety issue if minimum vacuum quality is limited to environmental atmospheric pressure and if full H_2 release from chemisorbed water is assumed. However, the computations in APPENDIX A demonstrate the importance of achieving a high vacuum quality on safety if no breakdown of the chemisorbed water is considered.	Low
Helium backfill pressure	Low	Case 1: + 1,892% (Overpressurization)	Low
Atmospheric pressure environment[f]	Medium	Case 1: +2,520% (Overpressurization)	Low
Gas and canister material temperature[g,h]	Medium	Case 1: +19% (based on computations in degree kelvin) (Overpressurization)	Medium

6. DISCUSSION

The bounding pressure evaluations of the 10 × 18 DOE Standard Canister loaded with 32 ATR ASNF elements indicate that the maximum achievable canister pressure remains at 391 psig (2,696 kPag),

[f]Studying the sensitivity of dry storage safety to the atmospheric pressure in the environment led to the following observation: The pressure of the DOE Standard Canister at gauge could increase with increasing atmospheric pressure, due to the fact that the helium backfill pressure is measured at gauge, too (which requires an increase in the amount of helium backfilled into the canister when the atmospheric pressure is high). Nevertheless, the impact of this effect on the conservatism of the base cases is insignificant: The base cases assumed a low atmospheric pressure of 0.5 atm and resulted in canister pressures of 391 and 251 psig [2,696 kPag and 1,729 kPag], in the 10 × 18 and 10 × 24 DOE Standard Canister, respectively. Under realistic upper limit conditions (i.e., an environmental pressure of <1.5 atm), the canister pressures under similar assumptions could increase to 400 and 261 psig [2,757 and 1,800 kPag], in the 10 × 18 and 10 × 24 DOE Standard Canister, respectively.

[g]Note that these sensitivity studies indicate canister overpressurization when reaching 316°C, which is below the Primary Service Temperature of 343.3°C defined in the preliminary design specifications of the DOE Standard Canister.

[h]Note that the level of control of the canister material temperature on the permissible canister pressure is lower than the level of control of the gas temperature on the actual canister pressure. While the increased gas temperature raises the canister pressure from 391 psig (2,696 kPag) at 220°C to 468 psig (3,226 kPag) at 316°C (i.e., by ~+20%), the permissible canister pressure decreases from 515 psig (3,553 kPag) at 220°C to 467 psig (3,219 kPag) at 316°C (i.e., by ~9%) due to material softening.

significantly below the permissible canister pressure of 515 psig (3,553 kPag). Thus, no structural integrity concerns were identified. The bounding flammability evaluations indicate the potential for sufficient H_2 buildup to exceed the 5% LFL by wide margins, reaching concentrations above 95%. However, the possible O_2 build up was insignificant, with the concentration remaining at 0.01%, which is significantly below the 4% LFL. Thus, no flammability issues were identified.

The bounding pressure evaluations of the 10 × 24 DOE Standard Canister loaded with 40 ATR ASNF elements indicate that the maximum achievable canister pressure remains at 251 psig (1,729 kPag), significantly below the permissible canister pressure of 515 psig (3,553 kPag). Thus, no structural integrity concerns were identified. The bounding flammability evaluations indicate the potential for sufficient H_2 buildup to exceed the 5% LFL by wide margins, reaching concentrations above 92%. However, the possible O_2 build up was insignificant, with the concentration remaining at 0.02%, which is significantly below the 4% LFL. Thus, no flammability issues were identified.

Sensitivity studies were conducted to identify DOE Standard Canister pressure and flammability controlling parameters. Qualitative levels of parameter uncertainty, paired with findings of studies on parameter value modifications needed, allowed identifying parameters that could control the safety of these ATR ASNF DOE Standard Canister configurations. Notably, no parameter with an associated “high” level of control was identified. However, several parameters, such as the free void volume of the canister after loading, the oxide layer thickness and associated properties (i.e., density and water content), and gaseous canister atmosphere and canister material temperatures received a “medium” rating, due to associated uncertainties and the limited value modification size to enable a safety issue. For example, studying the sensitivity of the canister pressure to variations in gaseous canister atmosphere and canister material temperatures indicates that a temperature increase to 316°C is sufficient to overpressurize the canister, which is above the predicted upper limit temperature of 220°C in the currently considered ASNF dry storage configurations, but below the DOE Standard Canister Primary Service Temperature of 343.3°C. Thus, it is recommended to consider significant modifications in the expected temperature, as well as in the expected values of all parameters with a medium level of control of canister pressure and flammability as safety relevant.

7. CONCLUSIONS

These evaluations represent bounding cases with regards to the pressurization and flammability of 10 × 18 and 10 × 24 DOE Standard Canisters loaded with DOE-managed ASNF. No structural integrity or flammability issues were identified. This aligns with our current understanding on the safety of extended ASNF dry storage (i.e., that the extended dry storage of U.S. DOE-managed ASNF in sealed systems is safe and technically feasible).

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APPENDIX A

Effect of Vacuum Quality on Flammability Control:

The targeted vacuum of 3 torr (400 Pa) at 25°C would, for void volumes of 211,035 cm^3 and 417,727 cm^3 in the loaded 10 × 18 and 10 × 24 DOE Standard Canisters, respectively, allow for approximately 0.03–0.07 mol of gas to reside within the canister. Assuming the hypothetical case of this gas being pure steam and that this steam undergoes a complete radiolytic breakdown during extended periods of sealed dry storage, oxyhydrogen with an H_2 to O_2 ratio of 2:1 could be created (see Assumption 2), increasing the quantity of gaseous species by a factor of 1.5. Thus, the maximum quantity of gaseous species due to imperfect canister evacuation would remain at around 0.1 mol or less, which could lead to insignificant partial gas pressure of <0.15 psi (~1 kPa) at 220°C. Further, note that the evaluations in this report indicate the possibility of relatively large amounts (>100 mol) of H_2 released from chemisorbed water, resulting in high H_2 concentrations above the established 5% LFL, thus making the contribution of H_2 from the radiolytic break down of steam insignificant. Furthermore, under the conservative assumptions of backfilling the canister with helium at the minimum credible pressure of 13.8 kpag at 21°C, a minimum credible atmospheric pressure of 0.5 atm (50.7 kPa) at 21°C, and a vacuum quality of 3 torr (0.4 kPa) at 25°C, the minimum amount of helium in the canister is ~5 mol, which limits the highest possible O_2 concentration (generated by the radiolytic breakdown of the residual steam in the canister) to ~0.3% (see an Table A1).

However, the impact of vacuum quality on canister safety can be easily demonstrated, too. The results in Table A1 indicate that an O_2 concentration above the 4% LFL appears possible if the vacuum pressure in a 10 × 18 DOE Standard Canister exceeds a pressure of ~41.3 torr. Note that these computations disregard any other sources (such as chemisorbed water) of H_2 that could reduce the resulting O_2 concentration in the canister atmosphere.

Table A1. Exemplary demonstration of the importance of vacuum quality on dry storage safety considering a 10 × 18 DOE Standard Canister configuration.

Backfill Pressure at 21°C	**Atmospheric Pressure at 21°C**	**Vacuum Pressure at 25°C**	**Partial Pressure of Helium at 21°C**	**Quantity of Helium in Canister**	**Quantity of Oxyhydrogen in Canister (2:1)**	**O_2 Concentration**
13.8 kPag	0.5 atm (50.7 kPa)	3 torr (0.4 kPa)	13.8 + 50.7 – 0.4 * 294.15 / 298.15 = 64.1 kPa	(64.1 * 1000 * 0.2111035) / (8.31446 * 294.15) = 5.5 mol	(400 * 0.2111035) / (8.31446 * 298.15) * 1.5 = 0.05 mol	(0.05 * 1 / 3) / (5.5 + 0.05) = 0.3%
13.8 kPag	0.5 atm (50.7 kPa)	41.3 torr (5.5 kPa)	13.8 + 50.7 – 5.5 * 294.15 / 298.15 = 59.1 kPa	(59.1 * 1000 * 0.2111035) / (8.31446 * 294.15) = 5.1 mol	(5500 * 0.2111035) / (8.31446 * 298.15) * 1.5 = 0.7 mol	(0.7 * 1 / 3) / (5.1 + 0.7) = 4%

APPENDIX B

Case 1:

06/04/2023 16:21:55

User Input:
- Canister Type: 10x18
- Canister Volume: 0.382974 m^3
- Canister Void Volume: 0.551 [-]
- Canister Corrosion: 0.1 [-]
- SNF Type: ASNF
- (Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
- (Oxy)hydroxide Layer Type: Trihydrate
- Total SNF Volume: 0.0 [m^3]
- SNF Porosity: 0.0 [-]
- Saturation of SNF Pores: 0.0 [-]
- SNF Surface Area: 115.2 [m^2]
- Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
- Number of Residual Water Layers on SNF Surface: 0 [#]
- Quantity of other Free Water in Canister: 0.0 [m^3]
- Residual and Free Water - Associated Temperature: 298.15 [K]
- Vacuum Drying Pressure: 399.9671052633 [Pa]
- Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
- Helium Backfill Pressure: 27600.0 [Pa]
- Helium Backfill Pressure - Associated Temperature: 294.15 [K]
- Environmental Pressure: 50662.5 [Pa]
- Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:
- Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
- Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

- Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
- Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 6.718561673071357 [mol]
- Molar Mass Water: 0.01801528 [kg/mol]
- Chemisorbed Water:
  - Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
  - Trihydrate Density at 25°C: 2430 [kg / m^3]
  - Trihydrate Water Content: 0.346 [-]
  - Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]
- Physisorbed Water: 0 [mol]
- Free Water: 0 [mol]

- Total Quantity of Gas in Canister: 0.05107018426806942 + 6.718561673071357 + 134.41070025000997 + 0.0 + 0.0 = 141.1803321073494 [mol]

Absolute Gas Pressure in Canister: (141.1803321073494 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 2743257.2270617695 [Pa]
Gauge Gas Pressure in Canister: 2743257.2270617695 - 50662.5 = 2692594.7270617695 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

2692594.7270617695 < 3553160.3240117338 -> Canister pressure check complete. No risk of overpressurization detected!

Computations complete!

Case 2:

06/04/2023 17:03:01

User Input:

Canister Type: 10x24
Canister Volume: 0.660416 m^3
Canister Void Volume: 0.633 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 144.0 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:

Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.660416 * 0.633 = 0.418043328 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.418043328) / (8.31446261815324 * 298.15) * 1.5 = 0.10117374632444609 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.418043328) / (8.31446261815324 * 294.15) = 13.309958914745136 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:

Trihydrate Volume: 2.5e-05 * 144.0 = 0.0036000000000000003 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 144.0 * 2430 * 0.346) / 0.01801528 = 168.01337531251247 [mol]

Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.10117374632444609 + 13.309958914745136 + 168.01337531251247 + 0.0 + 0.0 = 181.42450797358202 [mol]

Absolute Gas Pressure in Canister: (181.42450797358202 * 8.31446261815324 * 493.15) / 0.418043328 = 1779458.5657113707 [Pa]

Gauge Gas Pressure in Canister: 1779458.5657113707 - 50662.5 = 1728796.0657113707 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 10.001249999999999 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 294.79875 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.324011733 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.019367500000000003 [m]
Canister Head Sphere Radius, corroded: L = 0.607695 [m]
Canister Head Skirt Diameter, corroded: D = 0.5788025 [m]
Canister Head Knuckle Radius, corroded: r = 0.0385826 [m]
t/L = 0.03187042842215256 [-]
r/D = 0.06665935271530445 [-]
P/S = 0.04717232835409385 < 0.08:
ASME BPVC.III.3-2019 WC-3224.6-1: P_Head = 5024334.630553956 [Pa]

3553160.324011733 < 5024334.630553956 -> Maximum Allowable Canister Pressure: P = 3553160.324011733 [Pa]

1728796.0657113707 < 3553160.324011733 -> Canister pressure check complete. No risk of overpressurization detected!

Computations complete!

Case 1, 75% of Base Canister Void Volume:

08/04/2023 09:54:14

User Input:
Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.414 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 115.2 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:
Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.414 = 0.15855123599999998 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.15855123599999998) / (8.31446261815324 * 298.15) * 1.5 = 0.03837215297092693 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.15855123599999998) / (8.31446261815324 * 294.15) = 5.048066302452888 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:
Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]
Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.03837215297092693 + 5.048066302452888 + 134.41070025000997 + 0.0 + 0.0 = 139.4971387054338 [mol]

Absolute Gas Pressure in Canister: (139.4971387054338 * 8.31446261815324 * 493.15) / 0.15855123599999998 = 3607521.185762687 [Pa]

Gauge Gas Pressure in Canister: 3607521.185762687 - 50662.5 = 3556858.685762687 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

3556858.685762687 > 3553160.3240117338 -> Warning, the canister is of risk of overpressurization!

Computations complete!

Case 1, 134% of Base SNF Surface Area:

08/04/2023 10:13:33

User Input:
Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.551 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 154.0 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:
Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 6.718561673071357 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:
Trihydrate Volume: 2.5e-05 * 154.0 = 0.00385 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 154.0 * 2430 * 0.346) / 0.01801528 = 179.68097082032585 [mol]
Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.05107018426806942 + 6.718561673071357 + 179.68097082032585 + 0.0 + 0.0 = 186.45060267766527 [mol]

Absolute Gas Pressure in Canister: (186.45060267766527 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 3622898.144881909 [Pa]

Gauge Gas Pressure in Canister: 3622898.144881909 - 50662.5 = 3572235.644881909 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

3572235.644881909 > 3553160.3240117338 -> Warning, the canister is of risk of overpressurization!

Computations complete!

Case 1, 316% of Base Canister Corrosion:

08/04/2023 10:01:18

User Input:
Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.551 [-]
Canister Corrosion: 0.316 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 115.2 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:
Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 6.718561673071357 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:
Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]
Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.05107018426806942 + 6.718561673071357 + 134.41070025000997 + 0.0 + 0.0 = 141.1803321073494 [mol]

Absolute Gas Pressure in Canister: (141.1803321073494 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 2743257.2270617695 [Pa]

Gauge Gas Pressure in Canister: 2743257.2270617695 - 50662.5 = 2692594.7270617695 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 5.7007125 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 222.89928749999999 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 2689634.761896291 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0128651 [m]
Canister Head Sphere Radius, corroded: L = 0.4510151 [m]
Canister Head Skirt Diameter, corroded: D = 0.43781980000000004 [m]
Canister Head Knuckle Radius, corroded: r = 0.030797500000000002 [m]
t/L = 0.028524765578802132 [-]
r/D = 0.07034286708824042 [-]
P/S = 0.04078404103947828 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: P_Head = 4343916.802885587 [Pa]

2689634.76189629 < 4343916.802885587 -> Maximum Allowable Canister Pressure: P = 2689634.76189629 [Pa]

2692594.7270617695 > 2689634.76189629 -> Warning, the canister is of risk of overpressurization!

Computations complete!

<u>Case 1, 133 % of Base Oxide Layer Thickness:</u>[i]

08/04/2023 10:46:32

User Input:

Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.551 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 3.325e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 115.2 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:

Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 6.718561673071357 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:

Trihydrate Volume: 3.325e-05 * 115.2 = 0.0038304000000000003 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (3.325e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 178.76623133251329 [mol]

Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.05107018426806942 + 6.718561673071357 + 178.76623133251329 + 0.0 + 0.0 = 185.5358631898527 [mol]

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[i]Note that this sensitivity study case yields results representative for similar modifications in oxide layer density and water content.

Absolute Gas Pressure in Canister: (185.5358631898527 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 3605123.9572640997 [Pa]
Gauge Gas Pressure in Canister: 3605123.9572640997 - 50662.5 = 3554461.4572640997 [Pa]

Computations - Resistance:
Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:
Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:
Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

3554461.4572640997 > 3553160.3240117338 -> Warning, the canister is of risk of overpressurization!

Computations complete!

Case 1, Adding One Physisorbed Water Layer with 7 µm Thickness:

08/04/2023 10:50:42

User Input:
- Canister Type: 10x18
- Canister Volume: 0.382974 m^3
- Canister Void Volume: 0.551 [-]
- Canister Corrosion: 0.1 [-]
- SNF Type: ASNF
- (Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
- (Oxy)hydroxide Layer Type: Trihydrate
- Total SNF Volume: 0.0 [m^3]
- SNF Porosity: 0.0 [-]
- Saturation of SNF Pores: 0.0 [-]
- SNF Surface Area: 115.2 [m^2]
- Thickness of Residual Water Layers on SNF Surface: 7e-06 [m]
- Number of Residual Water Layers on SNF Surface: 1 [#]
- Quantity of other Free Water in Canister: 0.0 [m^3]
- Residual and Free Water - Associated Temperature: 298.15 [K]
- Vacuum Drying Pressure: 399.9671052633 [Pa]
- Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
- Helium Backfill Pressure: 27600.0 [Pa]
- Helium Backfill Pressure - Associated Temperature: 294.15 [K]
- Environmental Pressure: 50662.5 [Pa]
- Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:

Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 6.718561673071357 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:

- Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
- Trihydrate Density at 25°C: 2430 [kg / m^3]
- Trihydrate Water Content: 0.346 [-]
- Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]

Density of Water at 25.0°C: (999.83952 + 16.945176 * 25.0 - 7.9870401 * 10 ** -3 * 25.0 ** 2 - 46.170461 * 10 ** -6 * 25.0 ** 3 + 105.56302 * 10 ** -9 * 25.0 ** 4 - 280.54253 * 10 ** -12 * 25.0 ** 5) / (1 + 16.897850 * 10 ** -3 * 25.0 = 996.7294738665296 [kg / m^3]
Physisorbed Water:

- Quantity of Molecular Hydrogen Released from 1 Water Layers with a Thickness of 7.0 Microns on 1152000.0 cm^2 of SNF Surface Area: 7e-06 * 1 * 115.2 * 996.7294738665296 / 0.01801528 = 44.61560673639096 [mol]

Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.05107018426806942 + 6.718561673071357 + 134.41070025000997 + 44.61560673639096 + 0.0 = 185.79593884374034 [mol]

Absolute Gas Pressure in Canister: (185.79593884374034 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 3610177.454493215 [Pa]
Gauge Gas Pressure in Canister: 3610177.454493215 - 50662.5 = 3559514.954493215 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

3559514.954493215 > 3553160.3240117338 -> Warning, the canister is of risk of overpressurization!

Computations complete!

Case 1, Adding 235 ml of Free Water:

08/04/2023 11:32:12

User Input:
Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.551 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 115.2 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.000235 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:
Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 6.718561673071357 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:
Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]

Density of Water at 25.0°C: (999.83952 + 16.945176 * 25.0 - 7.9870401 * 10 ** -3 * 25.0 ** 2 - 46.170461 * 10 ** -6 * 25.0 ** 3 + 105.56302 * 10 ** -9 * 25.0 ** 4 - 280.54253 * 10 ** -12 * 25.0 ** 5) / (1 + 16.897850 * 10 ** -3 * 25.0 = 996.7294738665296 [kg / m^3]
Physisorbed Water: 0 [mol]
Free Water:
Quantity of Oxyhydrogen (2:1) Released from 235.0 ml of Free Water: 0.000235 * 996.7294738665296 / 0.01801528* 1.5 = 19.502729879188756 [mol]

Total Quantity of Gas in Canister: 0.051070184268069 42 + 6.718561673071357 + 134.41070025000997 + 0.0 + 19.502729879188756 = 160.68306198653815 [mol]

Absolute Gas Pressure in Canister: (160.68306198653815 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 3122212.311597465 [Pa]
Gauge Gas Pressure in Canister: 3122212.311597465 - 50662.5 = 3071549.811597465 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

3071549.811597465 < 3553160.3240117338 -> Canister pressure check complete. No risk of overpressurization detected!

Computations complete!

Case 1, Decreasing Vacuum Quality to Environmental Atmospheric Pressure:

08/04/2023 11:52:50

User Input:

Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.551 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 115.2 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 50662.500000018 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:

Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (50662.500000018 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 6.468890007288794 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 50662.500000018 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 2.440015124390874 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:

Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]

Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 6.468890007288794 + 2.440015124390874 + 134.41070025000997 + 0.0 + 0.0 = 143.31960538168963 [mol]

Absolute Gas Pressure in Canister: (143.31960538168963 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 2784825.1762434705 [Pa]

Gauge Gas Pressure in Canister: 2784825.1762434705 - 50662.5 = 2734162.6762434705 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

2734162.6762434705 < 3553160.3240117338 -> Canister pressure check complete. No risk of overpressurization detected!

Computations complete

Case 1, 1,992 % of Base Backfill Pressure:

08/04/2023 11:55:56

User Input:
Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.551 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 115.2 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 550000.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:
Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
Quantity of Backfill Helium: ((550000.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 51.79203441996252 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:
Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]
Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.05107018426806942 + 51.79203441996252 + 134.41070025000997 + 0.0 + 0.0 = 186.25380485424057 [mol]

Absolute Gas Pressure in Canister: (186.25380485424057 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 3619074.191195716 [Pa]

Gauge Gas Pressure in Canister: 3619074.191195716 - 50662.5 = 3568411.691195716 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

3568411.691195716 > 3553160.3240117338 -> Warning, the canister is of risk of overpressurization!

Computations complete!

Case 1, 2,620 % of Environmental Atmospheric Pressure:

08/04/2023 12:16:26

User Input:

Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.551 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 115.2 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 1327357.5 [Pa]
Maximum Canister Gas Temperature: 493.15 K

Computations - Demand:

Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
Quantity of Backfill Helium: ((27600.000000000073 + 1327357.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 116.87376322091251 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:

Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]

Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]

Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.05107018426806942 + 116.87376322091251 + 134.41070025000997 + 0.0 + 0.0 = 251.33553365519055 [mol]

Absolute Gas Pressure in Canister: (251.33553365519055 * 8.31446261815324 * 493.15) / 0.21101867400000002 = 4883669.055210674 [Pa]

Gauge Gas Pressure in Canister: 4883669.055210674 - 1327357.5 = 3556311.555210674 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603

Membrane Stress Intensity Limit at 220.0°C: Sm = 106510210.66501838 [Pa]

Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]

Membrane Stress Intensity Limit Sm = 106510210.66501838 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 106510210.66501838 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)

Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]

Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]

ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3553160.3240117338 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]

Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]

Canister Head Skirt Diameter, corroded: D = 0.433705 [m]

Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]

t/L = 0.03279832519190509 [-]

r/D = 0.06626647144948755 [-]

P/S = 0.04901448103974242 < 0.08:

ASME BPVC.III.3-2021 WC-3224.6-1: 5220542.701179515 [Pa]

3553160.3240117338 < 5220542.701179515 -> Maximum Allowable Canister Pressure: P = 3553160.3240117338 [Pa]

3556311.555210674 > 3553160.3240117338 -> Warning, the canister is of risk of overpressurization!

Computations complete!

Case 1, 144% of Gas/Canister Material Temperature:

10/04/2023 16:16:09

User Input:
Canister Type: 10x18
Canister Volume: 0.382974 m^3
Canister Void Volume: 0.551 [-]
Canister Corrosion: 0.1 [-]
SNF Type: ASNF
(Oxy)hydroxide Layer Thickness: 2.5e-05 [m]
(Oxy)hydroxide Layer Type: Trihydrate
Total SNF Volume: 0.0 [m^3]
SNF Porosity: 0.0 [-]
Saturation of SNF Pores: 0.0 [-]
SNF Surface Area: 115.2 [m^2]
Thickness of Residual Water Layers on SNF Surface: 0.0 [m]
Number of Residual Water Layers on SNF Surface: 0 [#]
Quantity of other Free Water in Canister: 0.0 [m^3]
Residual and Free Water - Associated Temperature: 298.15 [K]
Vacuum Drying Pressure: 399.9671052633 [Pa]
Vacuum Drying Pressure - Associated Temperature: 298.15 [K]
Helium Backfill Pressure: 27600.0 [Pa]
Helium Backfill Pressure - Associated Temperature: 294.15 [K]
Environmental Pressure: 50662.5 [Pa]
Maximum Canister Gas Temperature: 589.15 K

Computations - Demand:
Ideal Gas Constant: 8.31446261815324 [m^3 * Pa * K^-1 * mol^-1]
Canister Void Volume: 0.382974 * 0.551 = 0.21101867400000002 [m^3]

Quantity of Oxyhydrogen (2:1) Released from Residual Steam due to Imperfect Vacuum: (399.9671052633 * 0.21101867400000002) / (8.31446261815324 * 298.15) * 1.5 = 0.05107018426806942 [mol]
Quantity of Backfill Helium: ((27600.0 + 50662.5 - 399.9671052633 * 294.15 / 298.15) * 0.21101867400000002) / (8.31446261815324 * 294.15) = 6.718561673071357 [mol]
Molar Mass Water: 0.01801528 [kg/mol]
Chemisorbed Water:
Trihydrate Volume: 2.5e-05 * 115.2 = 0.00288 [m^3]
Trihydrate Density at 25°C: 2430 [kg / m^3]
Trihydrate Water Content: 0.346 [-]
Quantity of Molecular Hydrogen Released from Trihydrate: (2.5e-05 * 115.2 * 2430 * 0.346) / 0.01801528 = 134.41070025000997 [mol]
Physisorbed Water: 0 [mol]
Free Water: 0 [mol]

Total Quantity of Gas in Canister: 0.05107018426806942 + 6.718561673071357 + 134.41070025000997 + 0.0 + 0.0 = 141.1803321073494 [mol]

Absolute Gas Pressure in Canister: (141.1803321073494 * 8.31446261815324 * 589.15) / 0.21101867400000002 = 3277278.70895963 [Pa]

Gauge Gas Pressure in Canister: 3277278.70895963 - 50662.5 = 3226616.20895963 [Pa]

Computations - Resistance:

Material Properties derived from ASME BPVC.II.D.C-2021 Table 2A, 16Cr-12Ni-2Mo, Smls. pipe, SA-312, TP316L, S31603
Membrane Stress Intensity Limit at 316.0°C: Sm = 96493507.26948895 [Pa]
Stress intensity factor according to ASME BPVC.III.3-2021 Table WC-3217-1: k = 1.0 [-]
Membrane Stress Intensity Limit Sm = 96493507.26948895 multiplied by the Stress intensity factor k = 1.0 according to ASME BPVC.III.3-2021 WC-3224.2: S = 96493507.26948895 [Pa]

Canister Shell:

Manufacture Canister Shell Wall Thickness Tolerance: 12.5 [%] (ASME BPVC.II.A-2021 SA-312/SA-312M Table 3)
Minimum Canister Shell Wall Thickness, corroded: t = 7.500937500000001 [mm]
Maximum Canister Shell Inner Radius, corroded: R = 221.0990625 [mm]
ASME BPVC.III.3-2021 WC-3224.3 (a): P_Shell = 3219005.008195819 [Pa]

Canister Head:

Canister Head Wall Thickness, corroded: t = 0.0149225 [m]
Canister Head Sphere Radius, corroded: L = 0.45497750000000003 [m]
Canister Head Skirt Diameter, corroded: D = 0.433705 [m]
Canister Head Knuckle Radius, corroded: r = 0.0287401 [m]
t/L = 0.03279832519190509 [-]
r/D = 0.06626647144948755 [-]
P/S = 0.04901448103974242 < 0.08:
ASME BPVC.III.3-2021 WC-3224.6-1: P_Head = 4729579.1825186135 [Pa]

3219005.008195819 < 4729579.1825186135 -> Maximum Allowable Canister Pressure: P = 3219005.008195819 [Pa]

3226616.20895963 > 3219005.008195819 -> Warning, the canister is of risk of overpressurization!

Computations complete!