ABSTRACT

SRIMOK BOONCHAWEE. Investigation of Nuclear Waste Management for Advanced Fuel Cycles. (Under the direction of Man-Sung Yim).

Advanced nuclear fuel cycles (AFC), which are actively investigated by the U.S. Department of Energy, require advanced separation of spent nuclear fuels to recover uranium and other material of concern or interest. As these materials are being separated, issues such as how to manage these materials and the wastes associated with the processes must be addressed. Integrated Waste Management (IWM) Concept was proposed for this purpose. IWM not only focuses on material separations but also examines waste management strategy to support the AFC. Many factors, such as volume of waste to be disposed, radiation dose and cost, are considered in optimizing the waste management strategy. In order to study the feasibility of the IWM concept, a thorough investigation must be performed.

The objective of this research is to perform a detailed examination on the waste management strategies form advanced separation processes utilized in the AFC. To achieve this goal, a computer code named Integrated Waste Management Simulation (IWMS) was developed. Tasks include: (1) approximation of the amount of individual nuclear wastes streams derived from the advanced separation process; (2) suggestion of the best waste management option for each stream, according to their inherent characteristics, such as radioactivity concentration, volume of final waste forms and radiation dose; and (3) estimation of the associated costs of the entire separation processes, as well as all corresponding waste treatment and handling processes.

The IWMS code was developed and successfully demonstrated by utilizing the UREX process as a case study. Due to the limited availability of the information needed for the analysis, assumptions were made using available data in order to demonstrate the code's capabilities. Sensitivity study on the UREX process input parameters, i.e. advanced

separation processes costs, waste form manufacturing costs, waste disposal cost, decision weights and others, was also performed. The sensitivity study indicated that the results were sensitive and subject to the major input parameters being used. These findings suggested that the IWMS code could be useful to perform various studies, such as analyzing the waste management strategies of the UREX process against the UREX+ process or the UREX+1 process with the UREX+1A process.

Investigation of Nuclear Waste Management for Advanced Fuel Cycles

by
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BIOGRAPHY

Boonchawee Srimok, daughter of Pon Srimok and Boonsom Srimok, was born in Ayudthaya, Thailand, on December 2, 1972. In 1993, she earned her B.Sc. in Industrial Chemistry from the department of Chemistry, faculty of Science of King MongKut Institute of Technology at Ladkrabang. In the same year, she continued her study at Chulalongkorn University in the Department of Nuclear Technology, from which she received her M.E. in Nuclear Technology in 1997. She began her career as a nuclear chemist in the Office of Atomic Energy for Peace (which has now become the Office of Atoms for Peace), Bangkok, Thailand in 1997. In 2004, she was awarded a full scholarship from the Royal Thai Government to continue her graduate studies in the Nuclear Engineering Department at North Carolina State University.

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Chapter 1 Introduction

Nuclear power is one of the leading energy sources that demonstrate low carbon dioxide emissions. Ensuring a sustainable development of nuclear power in response to a gradual global growth of electricity generation requires an effective nuclear fuel cycle.

1.1 Nuclear Fuel Cycle

Nuclear fuel cycle is defined as a series of processes that involve a production of electricity using nuclear power. It includes all of the processes from uranium mining, uranium conversion, to fuel enrichment and fabrication, fuel irradiation in the reactor, irradiated fuel or Used Nuclear Fuel (UF) storage and disposal. Two types of cycles (Figure 1-1) are generally adopted by nuclear power countries: closed fuel cycle and opened fuel cycle. The opened fuel cycle can also be called “once-through cycle”. While countries such as France, Japan, United Kingdom, Russia and India adopted the closed cycles, the United States, Canada, Sweden and Finland chose the open ones. The major difference between the two cycles is that the once-through cycles require a direct permanent disposal of UF in a designated geologic repository, while closed cycles require UF reprocessing to retrieve usable material such as Uranium (U) and Plutonium (Pu) and the disposal of the remaining fission products in the designated geologic repository.

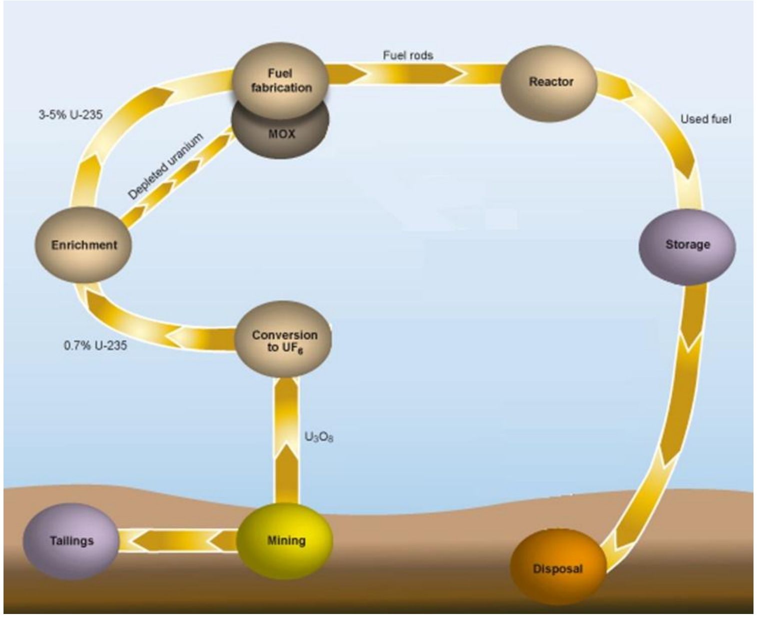

Figure 1-1a Once-Through Cycle

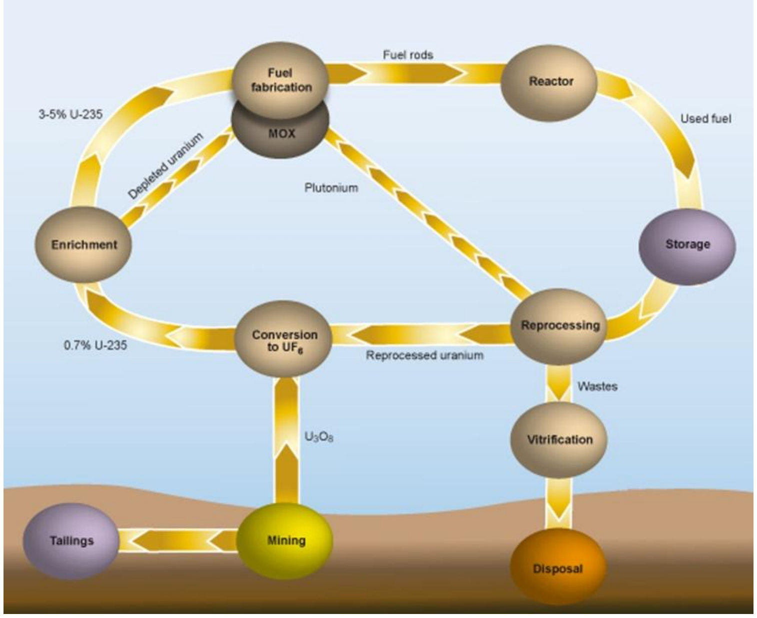

Figure 1-1b Closed-Fuel Cycle

Figure 1-1 Conventional nuclear fuel cycles

In the U.S., the only designated geologic repository is the Yucca Mountain Facility, (YMF), located in Nye County, NV. The YMF is limited by legislation to a maximum capacity of 70,000 metric tons of heavy metal (MTHM), of which 63,000 MTHM and 7000 MTHM are reserved for civilian and federal UF respectively. The civilian capacity limit is significantly less than the anticipated total UF expected to be generated in the U.S. soon, as illustrated in Figure 1-2. An immediate response to this situation is needed.

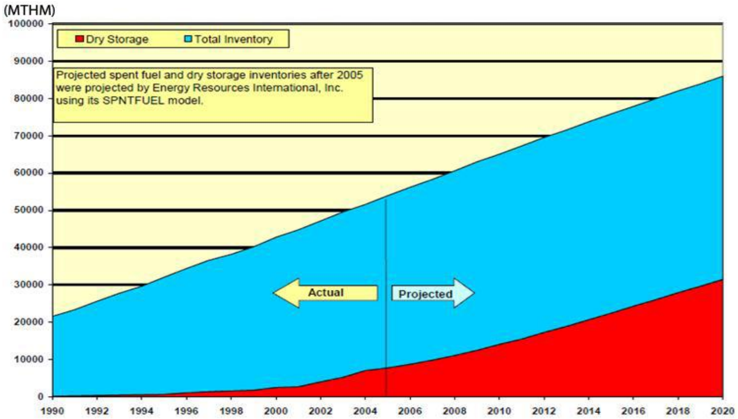

Figure 1-2 Projected used nuclear fuel and dry storage inventories

Because UF contains highly radioactive fission and activation products, a situation which results in heat generation, most UF is usually kept in a temporary storage pool for cooling awaiting a management solution at locations where the UF is generated. Although temporary storage at the power plant site could serve as a temporary solution to the capacity shortage, that is considered a non-permanent solution. As an alternative to the once-through cycle and a traditional closed nuclear fuel cycle, Advanced Fuel Cycle (AFC), which requires reprocessing of UF, was proposed [1] in order to separate: (1) usable material, such as Uranium (U), (2) short-term heat generator such as Cesium (Cs)/ Strontium (Sr), and (3) long-term dose contributor such as Neptunium (Np) and Technetium (Tc). Retrieving these elements is often done by aqueous separation by means of a solvent extraction process. Examples of these processes are: Plutonium Extraction process (PUREX), Uranium Extraction Process (UREX), Chlorinated Cobalt Dicarbollide/Poly Ethylene Glycol process (CCD/PEG), Transuranium extraction process (TRUEX) and Trivalent Actinide and

Lanthanide Separation by Phosphorus reagent Extraction from Aqueous Komplexes (TALSPEAK).

1.2 Advanced Fuel Cycle (AFC)

In AFC, advanced aqueous separation, often referred to as the employment of sequential individual solvent extraction processes, was planned to sequentially separate out elements of concern. In theory advanced separation process should reduce the amount of radionuclides of concern for disposal as the process is designed to recover useable material for reuse. Figure 1-3 shows the concept for the AFC compare to traditional closed fuel cycle.

Although feasibility of this advanced separation process has been studied, in order to support its implementation, a thorough investigation must be performed including cost analysis and process optimization. The basis for the cost of the advanced fuel cycle has been previously researched [2-4]. That research work did not focus on the detail of one important issue--the waste management of the plan. Idaho National Laboratory (INL) staffs led by D. Gombert proposed a methodology to address this waste issue for the back end part of the AFC, i.e. UF management processes [5]. This method is called “Integrated Waste Management (IWM),” and it attempts to find the most efficient technique that would address technological, economical, and social concerns, to treat all derived streams from UF reprocessing from their origins to disposals.

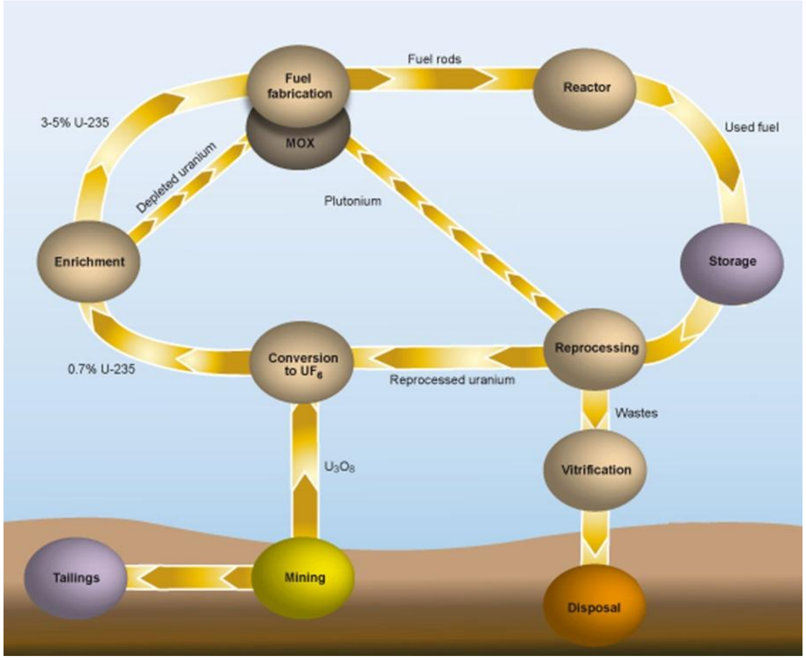

Figure 1-3a Closed Fuel Cycle

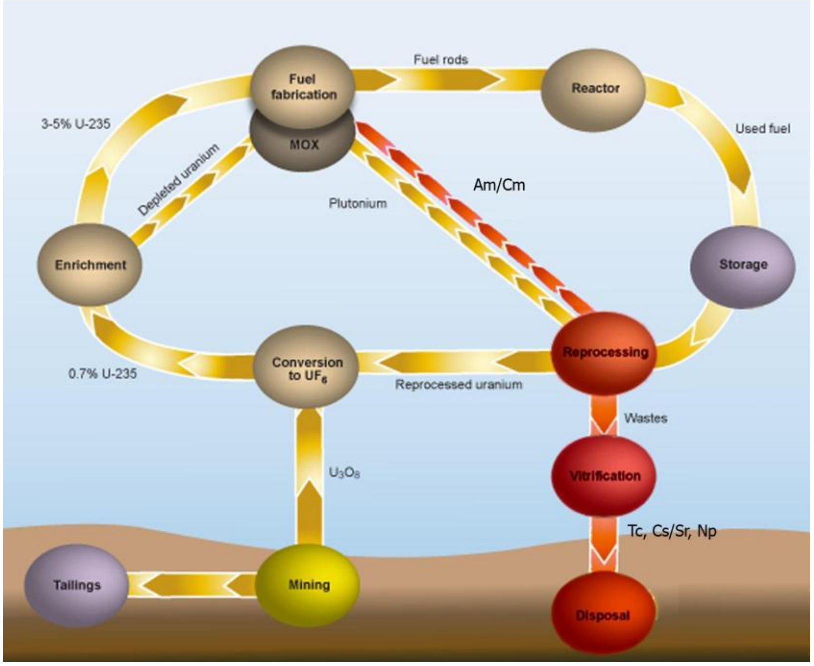

Figure 1-3b Advanced Fuel Cycle

Figure 1-3 Nuclear fuel cycles

1.3 Integrated Waste Management (IWM)

Opened-fuel or once-through cycle is a current national policy for UF management. As illustrated earlier, since the constitutional capacity at the only designated geologic repository, YMF, has been exceeded, a decision on either increasing this capacity or searching for a second geologic repository has to be made. Considering the long history of the YMF, it is more likely that the current capacity at the YMF would be increased than that a second geologic repository program would be initiated. The two most important limiting parameters for the YMF loading capacity are temperature (at various locations in UF container, drift walls, etc.) and long term radiation doses. Extensive research has been performed to demonstrate that removing some decay heat contributed radionuclides (e.g. Cs/Sr as short term heat contributors and Am/Cm as long term heat contributors) as well as the dose contributors can increase the YMF loading capacity significantly. Typical separation of the radionuclides from UF is through reprocessing by means of aqueous separation processes. In this particular case, separation of Cs/Sr and Am/Cm can be done by employing two aqueous separation processes simultaneously which corresponds to the AFC method mentioned in the previous section. However, adoption of the AFC concept, which typically incorporates UF separation, fuel refabrication, usable material recycling, and waste handling processes, can be quite challenging since most of the advanced separation processes are in the laboratory development stage. Unlike the PUREX process which is the baselines technology for reprocessing activities worldwide with well characterized waste management activities, radioactive waste associated with advanced separation employed in the AFC is not known. The IWMS code is primarily designed to ensure that all wastes generated from AFC will have an appropriate disposition path by taking advantage of the materials separation to eliminate or minimize byproducts and wastes. If waste must be generated, processes will be designed with waste treatment in mind both to reduce the use of reagents that complicate stabilization and to minimize volume. Quantification of all the wastes arising from all the relevant processes is a key to the IWM concept. In practice, not only the total amount of radioactive wastes generated from the AFC (separation, fuel fabrication and relevant processes) but also other parameters such as costs, occupation doses and doses to the public should be taken into account in IWM analysis.

As IWM extends the focus beyond the material separation, it also examines waste management strategy to support the AFC. Figure 1-4 illustrates this strategy. As shown in Figure 1-4, UF reprocessing by means of advanced separation is required. In this research, an advanced separation process shown in Figure 1-5 was proposed based on the current U.S. separation baseline (UREX+). Flow diagram and derived streams associated with this separation scheme are also shown in Figure 1-5.

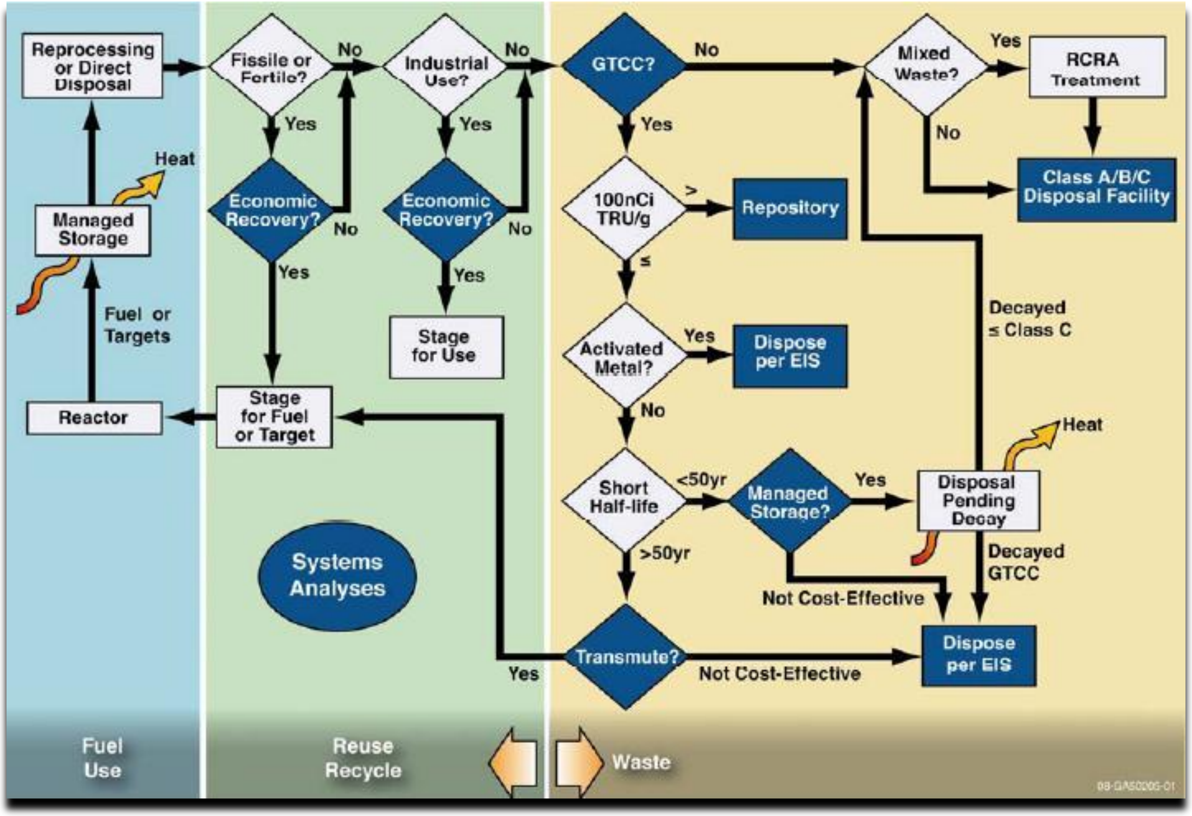

Figure 1-4 Integrated Waste Management (IWM) concepts[a]

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[a] http://www.engconfintl.org/9arIWMS.pdf

To allow an optimization study for the UF reprocessing, different combinations of head-end, separation and re-fabrication processes can be specified and corresponding estimates of system performance, such as associated costs and the amount of generated waste can be correspondingly determined.

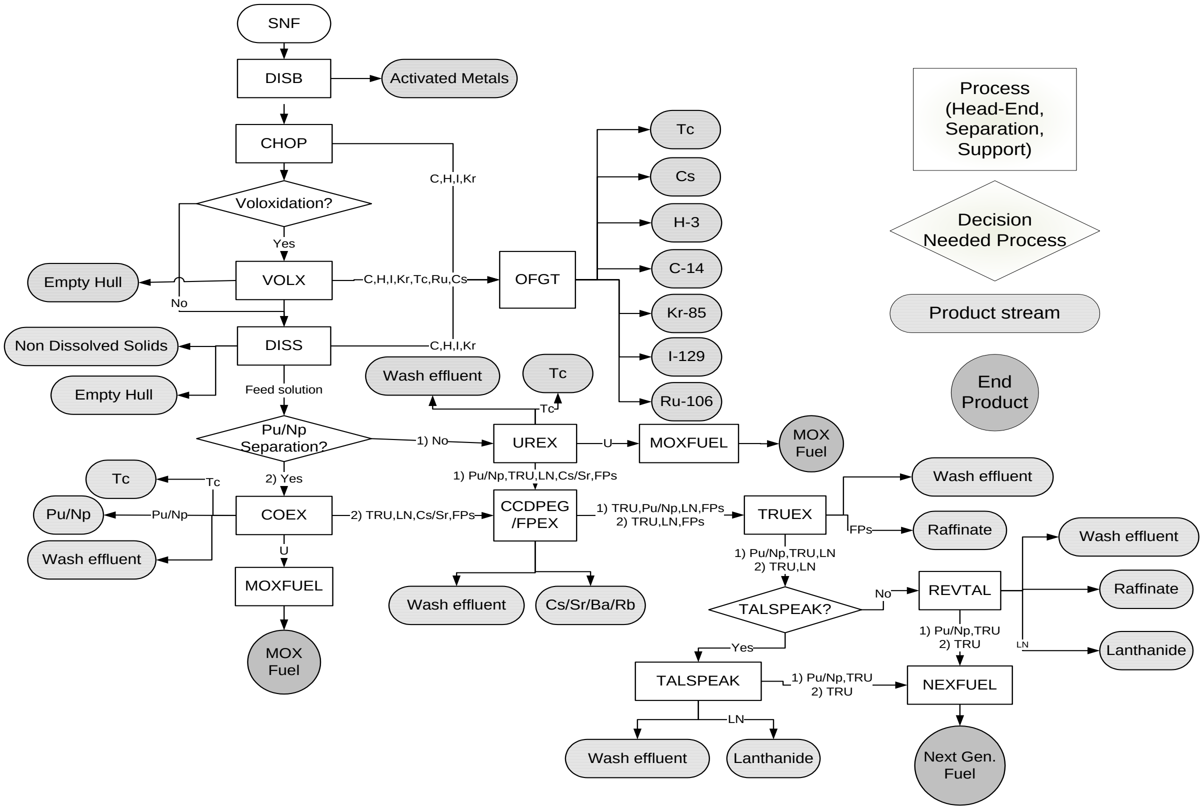

Figure 1-5 Simplified diagram of advanced separation in IWMS code

As seen in Figure 1-5, the advanced aqueous separation results in multiple streams with unique characteristics; some contain, a single element, some contain multiple radionuclides, some are composed of usable materials, some have a relatively high radioactivity level, some have a long half-life while most of them have short radiological half-life, etc. These properties depend on the irradiation history of an incoming UF being reprocessed. These characteristics also dictate how the product streams should be managed. Based on the IWM methods laid out in Figure 1-4, five management alternatives were proposed for the treatment of derived streams. They are: 1) exempts; 2) direct disposal; 3) transmutation; 4) decontamination and reuse and; 5) decay storage. In order to select the best management alternatives, a more detailed investigation of the waste management strategy must be performed. Several related studies have been conducted to address this issue [6 ,7]. One example is an Advanced Fuel Cycle modeling tool [7], as a simplified excel spreadsheet for nuclear fuel simulation of different types of the nuclear fuel cycle. In that work, reprocessing was assumed as a black box, i.e. the amount of waste produced and the costs associated with UF processing were constants, regardless of the target recovery efficiencies set at the beginning. The amount of nuclear waste associated with the UF reprocessing as a function of the key radionuclides recovery efficiencies is needed for a better waste management scheme as a whole, especially for the IWM scheme.

1.4 Objectives and Scope of Research

The goal of this research was to investigate management strategies for radioactive wastes from the advanced aqueous separation processes to support the Advanced Fuel Cycle. Tasks include (1) approximation of the amount of individual nuclear wastes streams derived from the advanced separation process; (2) suggestion of the optimum management option for each stream, according to its inherent characteristics, according to their inherent characteristics, such as radioactivity concentration, volume of final waste forms and radiation dose; and (3) estimation of the associated costs of the entire separation processes, as well as all corresponding waste treatment and handling processes. To perform the tasks and to achieve the goal, a computer code named Integrated Waste Management Simulation (IWMS) was developed, based on a current U.S. baseline separation process, i.e. UREX+, and the assumption that certain level of elemental separation efficiencies can be achieved during UF reprocessing.

Chapter 2 Literature review

Integrated Waste Management (IWM) involves UF reprocessing via aqueous separation and waste management which typically combines handling methodology and disposal. This section provides discussions of a current reprocessing technology and descriptions of the processes involved, i.e. summary of the head-end, separation and support processes of interest, particularly for the ones that support IWM; and waste management methodology.

2.1 UF reprocessing

Fuel discharged from a nuclear reactor after irradiation to the end of its useful life, or UF, still contains most of the fertile material (U-238) that was present in the fresh fuel, as well as fissile nuclides (U-235, and Pu) and/or and large amounts of radioactive, neutron-absorbing fission products. The principal objectives of reprocessing are: (1) to recover uranium and plutonium, and thorium if present, for reuse as nuclear fuels; (2) to remove radioactive and neutron-absorbing fission products from them; and (3) to convert the radioactive constituents of used fuel into forms suitable for safe, long-term storage. There may be some interest in recovering individual fission products such as Cs and Sr for use as radiation sources or in recovering by-product transuranic elements such as Np, americium (Am), or curium (Cm)[8]. The two types of UF reprocessing processes are: non-aqueous and aqueous methods. While the non aqueous method has been demonstrated to be a viable reprocessing technology on a laboratory scale [9-11], the aqueous method, such as the PUREX process, has been shown to be a mature technology that has been commercially applied in France, the UK and Japan. The overall aqueous process involves (1) head end, also known as pre-separation process, such as UF chopping/downsizing, and UF dissolution in nitric acid solution; (2) separation process via solvent extraction process, such as PUREX, which involves UF dissolution and selective separation of U and Pu from the rest of the radionuclide inventories dissolved in the UF solution. In current global nuclear security regime, extraction of Pu is considered to potentially increase the possibility of nuclear proliferation as accumulation of separated Pu increases the theoretical probability of diversion for military purposes. As a result, UREX, as opposed to PUREX, was selected as a baseline separation process in the U.S. as reflected in part of the U.S. nuclear policy. Despite small difference in the primary elements of separation, the remaining needs and process characteristics such as pre-separation process (head-end) and chemicals used for the separation process are quite similar. Preventing extraction of Pu (at the back-end of the nuclear fuel cycle) is not the only requirement needing to be effectively managed. Other requirements such as selective separation of radionuclides of concerns need to be addressed as well. The following section summarizes the steps required in reprocessing.

2.1.1 Head-End Process

The head-end process starts by de-structuring of cooled UF assembly into individual fuel rods and structure materials. The fuel rods contain most of the fission products (FP) and activation products, and the structure materials contain mostly activation products. The fuel rods are sent to the chopping/shredding process and the resulting chopped out fuel rods and hulls are dissolved in the dissolution process. During the head-end process, fission gas is often separated to prevent a complication in the separation process which is the next step.

Fission gas includes tritium gas, radioactive idodide, xenon and carbon dioxide gas. These gaseous species must be treated before they either are released into the environment or are contained and disposed of.

2.1.1.1 Voloxidation

Voloxidation is a process of oxidizing chopped/shredded fuel at up to 600°C in a rotary kiln to liberate volatile fission products into a small gas stream for simplified management [12]. Although the process has not been developed commercially, extensive laboratory scale research has been co-performed at Oak Ridge National Laboratory (ORNL) and Korean Atomic Energy Research Institute (KAERI). The process was designed to separate both volatile radionuclides (such as H-3, I-129, C-14 and Kr-85) and certain semi-volatile materials (such as Tc, Cs, Molybdenum (Mo) and Ruthenium (Ru)), prior to the dissolution process [13 ,14]. According to the research, more than 99 % of the volatile materials were reported to escape from the fuel. In case of semi-volatile materials, the released fractions were varied depending on the temperature used and the chemical forms of the semi-volatile elements in the UF. Another advantage of the voloxidation process is that the oxidized fuel powder is usually dissolved faster than fuel hulls. The drawback is that it has only been done in laboratory.

2.1.1.2 Dissolution

The objectives of fuel dissolution are (1) to bring the uranium and plutonium in the fuel completely into aqueous solution; (2) to complete the separation of fuel from fuel clad; (3) to determine as accurately as possible the amounts of uranium and plutonium charged to reprocessing; and (4) to convert uranium, plutonium, and fission products into the chemical states most favorable for their subsequent separation [8].

Because the separation process requires that the elements to be separated be present in aqueous solution as nitrates, the dissolvent is always nitric acid. The principal reactions that take place are:

$$3UO_2 + 8HNO_3 \rightarrow 3UO_2(NO_3)_2 + 2NO + 4HO_2$$

and

$$UO_2 + 4HNO_3 \rightarrow UO_2(NO_3)_2 + 2NO_2 + 2HO_2.$$

Normally, both reactions take place to some extent, with the first reaction dominant at acid concentrations below 10 M and the second at higher concentrations [8]. In principle, formation of gaseous reaction products could be avoided by the addition of oxygen directly to the dissolver:

$$2UO_2 + 4HNO_3 + O_2 \rightarrow 2UO_2(NO_3)_2 + 2HO_2.$$

This process is known as "fumeless dissolving" and is used in European plants. Practically, small amounts of nitrogen, nitrogen oxides, and gaseous fission products are also formed [8].

Plutonium in oxide fuel dissolves as a mixture of tetravalent and hexavalent plutonyl nitrates, both of which are extractable with TBP. Neptunium dissolves as a mixture of inextractable pentavalent and extractable hexavalent nitrates. Most of the fission products go into aqueous solution. However, at high burnups, some elements such as Mo, zirconium (Zr), ruthenium (Ru), rhodium (Rh), palladium (Pd), and niobium (Nb) may exceed their solubility limits and be present as solids.

The chemical forms in the solution of most of the fission product elements have not been extensively investigated as the Pu and U have been. There is an experiment on measuring both of the soluble and non-soluble fission product amounts in the solution has been performed [15]. This dissolution experiment used an actual UF, and reported the distribution of elements in fuel solution, fuel cladding and non-dissolved solid.

After reaction of the fuel with acid has been completed, the resulting solution and any non-dissolved particles are drained from the coarser cladding fragments. The cladding is washed, first with dilute nitric acid and then with water. The cladding is checked to establish removal of adherent fuel and then is normally discharged for packaging as radioactive waste. The fuel solution, possibly containing suspended particles, is clarified by centrifugation. Centrifuged solids are accumulated and periodically leached as described above for recovery of the elements of interests.

2.1.2 Separation Process

2.1.2.1 UREX

The UREX (Uranium Extraction) process [16 ,17] has been developed under the US Advanced Fuel Cycle Initiative (AFCI) program, with the aim of providing a process for fuel recycling which does not result in the separation of Pu explicitly. The process aims to recover >99.9 % of the U and >95 % of the Tc in separate product streams while rejecting >99.9 % of the TRU isotopes to the UREX raffinate stream. A mixture of 30% Tri-n-butyl phosphate (TBP) as extractant, in normal paraffin such as Dodecane was used to extract U and Tc into organic phase. The TBP mixture is retained as the principal organic solvent, but to avoid a separate Pu stream, the process was designed to use aceto-hydroxamic acid (AHA) in the scrub stream which chemically interacts with Pu (IV) and Np (IV), preventing them from extracting, and reduces Np (VI) to inextractable Np (V).

The UREX process has been demonstrated at the laboratory scale at the Savannah River National Laboratory in the USA, using irradiated fuel from the Dresden BWR[16]. According to the demonstration, the U losses to the Tc and raffinate streams were less than 0.02%, and the Tc losses to the U stream were < 1.2% and losses to the raffinate were low. This demonstrated that >95% of the Tc could be recovered. Loss of Pu and other actinides to the Tc and U product streams was <0.02 % in all tests, with >99.98 % going to the raffinate. UREX is considered to represent a modest change to the well-established PUREX technology, and has been adequately researched and demonstrated in the U.S.

2.1.2.2 COEX

An alternative route that is deployable in the short term is the COEX process which is an evolution of the PUREX process. COEX, or so-called co-decontamination process, was co-developed by CEA and AREVA and never requires separation or purification of pure plutonium. COEX uses the same extractant and diluents as the PUREX process, i.e. TBP in n-Dodecane system. In the first cycle, U, Pu, Np and Tc are all extracted into an organic phase. In the second step, both Pu and Np are selectively stripped (back extracted) from the loaded organic solvent by nitric acid solution and will remain in the same stream. Next, U and Tc are simultaneously stripped into the aqueous phase for further processing. A similar separation process was implemented at Argonne National Laboratory (ANL) as a UREX+2 process with the first solvent extraction process being the COEX process followed by Cs/Sr extraction process and TALSPEAK process in sequence. UREX+2 has been successfully demonstrated using actual UF [18]. In this test, the raffinate from prior a solvent extraction process was not continuously flowed to the next step process due to a limitation in laboratory space for the hot test.

2.1.2.3 CCD-PEG

A Chlorinated Cobalt Dicarbollide (CCD)/PolyEthylene Glycol (PEG) based solvent extraction process was first developed for the separation of Cs and Sr from UF solution at Idaho National Loboratory (INL) for supporting Fuel Cycle Initiative (AFCI)[19 ,20]. The solvent consists of 0.08 M CCD for the extraction of Cs, 0.6 vol% PEG-400 for the extraction of Sr, 0.02 M diphenyl-*N*,*N*-di-*n*-isobutylcarbamoyl-methylphosphine oxide (CMPO) for the extraction of the actinides and rare earth elements, and a phenyltrifluoromethyl sulfone (FS-13) as diluents. Only laboratory batch contact tests were performed using the CCD/PEG solvent. This process was designed to take UREX rafiinate and simultaneously extract Cs and Sr.

2.1.2.4 FPEX

Fission Product Extraction (FPEX) [21] is the process that consists of 4,4’,(5’)-di-(t-butyldicyclo-hexano)-18-crown-6 (DtBuCH18C6) to selectively extract Cs, calix[4]arene-bis- (tert-octylbenzo-crown-6) (BOBCalixC6) to extract Sr, and 1-(2,2,3,3-tetrafluoropropoxy)-3-(4-sec-butylphenoxy)-2-propanol (Cs-7SB modifier) in a branched aliphatic kerosene (Isopar@L) as diluents.

2.1.2.5 TRUEX

TRUEX [22] is an extraction process in which a mixture of Octyl(phenyl)-N,N-dibutylcarbamoyl Methyl Phosphine Oxide (CMPO); TBP; and normal paraffinic hydrocarbon (NPH), or, when there is a concern about fire or explosion prevention, a chlorocarbon, such as tetrachloroethylene (TCE), is used to separate the TRU fraction from acidic fuel solutions. The concentration of CMPO and TBP in the TRUEX-NPH solvent is 0.2 M and 1.4 M, respectively. The TRUEX-TCE solvent is formulated as 0.25 M CMPO and 0.75 M TBP diluted by TCE. The process has been demonstrated to work well at the laboratory scale [23 ,24], but pilot-plant demonstration has not been performed. An unanswered question about the TRUEX process that may limit its applicability involves separation of trivalent lanthanides from the trivalent transplutonium elements.

The extracting agents in the TRUEX, a carbamoyl methyl phosphoryl derivative and crown ether, respectively, have yet to be manufactured on a production scale, as will be needed if these processes are to be used for large-scale processing of UF. Among the issues to be addressed are (1) effective precursors and processing methodology for manufacturing the extractants; (2) the purity achievable; (3) the nature and chemical effects of impurities; (4) radiolytic and chemical stability; (5) solubility in water or losses to emulsification, sorption onto suspended impurities, etc. and (6) regenerability and degree of regeneration achievable. These factors could result in problems that would jeopardize use of the TRUEX process and therefore they require prompt evaluation. At present, TRUEX seems to be the most promising post-UREX (or COEX) technology for TRU isolation from UF.

2.1.2.6 TALSPEAK

The TALSPEAK process was first described in a report from Oak Ridge National Laboratory (ORNL)[25]. This process is based on separation of lanthanides from trivalent actinides by extraction of the trivalent actinides into di (2-ethylhexyl) phosphoric acid (HDEHP) organic phase from the aqueous phase of lactic and Diethylene Triamine PentaAcetate (DTPA) acids at pH 2.5 to 3.0. The mixture of carboxylic acid buffer and a DTPA is principally responsible for holding back the trivalent lanthanides, allowing the selective transfer of the actinides into the organic phase. This process has been demonstrated at the pilot scale using actual UF and process stimulants [26]. Various aspects of the process have been thoroughly reviewed [27]. In the context of the UREX process, TALSPEAK represents a process operation challenge, as it relies on a unique aqueous medium and an organic extractant that is not used elsewhere in the processing of the dissolved UF. Careful conditioning and preparation of feeds and extractants will be needed.

2.1.2.7 Reverse TALSPEAK

In principle, both TALSPEAK and reverse TALSPEAK [28] are based on the extraction of lanthanides using HDEHP from a medium that selectively retains the actinides in the aqueous phase as complexes with polyaminopolyacetic acid complexants such as DTPA. In the "reverse" TALSPEAK process, both of the trivalent actinide and lanthanide elements are extracted in an organic phase by HDEHP. Next the +3 metals are stripped into an aqueous phase of lactate and DTPA. Subsequently, 6 M nitric acid is used to strip the lanthanides. In the context of the UREX process, reverse TALSPEAK process takes raffinate from previous process as is, extracts both actinides and lanthanides into the organic phase, and strips lanthanides using DTPA in lactic acid buffer. This eliminates feed adjustment which seems to allow the continuous process if desired. This process was also demonstrated at a pilot scale at ORNL using mixer settler[29].

Table 2-1 Summary of Aqueous Separation Processes Chemicals

Process	Target Element	Solvent/Diluents	Extracting Agent	Stripping Agent	Status	Equipment
UREX[16]	U/Tc	n-Dodecane/ Kerosene	TBP	0.01 M HNO_3/ 10 M HNO_3	Countercurrent tested (Hot)	Centrifugal Contactor
CCD/PEG [30]	Cs/Sr	FS-13	CCD/PEG	Guanidine carbonate/ DPTA	Batch tested	NA
FPEX[21]	Cs/Sr	Aliphatic Hydrocarbon Diluent/Isopar® L	DtBu18C6/ BOBCalixC6	Dilute HNO_3	Batch tested	NA
TALSPEAK [26]	Trivalent Actinides & Lanthanides	NA	HDEHP	DTPA in 1 M citric acid	Countercurrent tested (Hot)	Mixer Settler
Reverse TALSPEAK[29]	Trivalent Actinides & Lanthanides	NA		DTPA in 1 M citric acid	Countercurrent tested (Hot)	Mixer Settler
TRUEX[23 ,24]	TRU	NPH/TCE	CMPO	1) 0.02- 0.05 M HNO_3 2) 0.04- 0.1M Hydrofluoric acid(HF)/ 0.05 M HNO_3	Countercurrent tested (Hot)	Centrifugal Contactor
COEX (ANL) [18]	U/Tc/Pu/Np	NPH/n-Dodecane/Kerosene	TBP		Countercurrent tested (Hot)	Centrifugal Contactor

2.1.3 Fuel Fabrication Process

2.1.3.1 Mixed Oxide (MOX) Fuel Fabrication

Plutonium (Pu) and Uranium (U) have been recycled in the form of MOX fuel in thermal reactors (essentially LWRs) for more than thirty years. A commercial application of MOX fuel in Light Water Reactors (LWRs) has been around since 1980s. Currently, the use of MOX fuel has been established on an industrial scale in a number of countries such as Belgium, France, Germany, Japan, UK and Switzerland. MOX fuel fabrication technologies were developed and are considered mature. MOX fuel fabrication generally composes of: (1) conversion of Pu and U into oxide form and (2) manufacture of these mixture oxides into MOX fuel. Although a number of methods have been used to prepare Pu and U of different form into oxide, the most common initial form for both elements is the nitrate form as a product of the PUREX process. The focus here is the conversion from the nitrate form. Common technologies that serve the purpose include; precipitation of plutonium oxalate [31], thermal de-nitration[32], co-precipitation[33] and gel precipitation methods[34]. Summary details can be found in Ref [35]. For the manufacturing of MOX fuel, common methodologies are: MIcronized MASter blend or MIMAS[36]; CObroyage (co-milling) CAdarache or COCA; Vipac; Short Binderless Route or SBR; and conventional methods. Summary details can be found in Ref [35].

In the development of IWMS, a thermal de-nitration conversion method and the French fabrication method (COCA) were used as a basis for MOX fuel fabrication modeling. Since in this research UREX+ is the primary focus, most of the modeling assumed that Pu is fed from a source outside the IWMS scheme, i.e. Pu from the stockpile. Only U from UREX process is fed to MOX fuel fabrication.

2.1.3.2 Next Generation Fuel Fabrication

Fuel fabrication for the next generation reactor, sometimes called fast reactor (FR), usually involves minor actinide (MA), i.e. Am or Cm, as raw material in the fuel. At the present time, no industrial scale plant has the capability to do so. Summary reviews of the research on minor actinide fuel were found in Ref [37 ,38].

Since the completed design of the next generation reactor is still not revealed, the exact fuel design that will be used in it is still uncertain in nature. The only thing that could be relied on in the fabrication of the MA-fuel is the experience from the FR MOX fuel fabrication facilities, although with the caveat that a higher content of Pu and a large amount of Americium (Am) used in MA fuel production will require a remotely operated production line. Novel methods such as sol-gel, infiltration and vibropack were suggested [38]. The sol-gel process was used as a model in IWMS.

2.1.4 Off-Gas Treatment Process

As UF is chopped during head-end process and advanced to the solvent extraction process in the later steps, fission gas is released from various processes including the chopping process and the dissolution process. The off-gas released during dissolution process is usually referred to dissolver off gas (DOG), and the off-gas released in the later step is called vessel off gas (VOG). DOG is the majority (about 80-90 percents) of the off gas compared to the total VOG combined for the rest of the processes. Among many fission gas species, several are of concern in different situations, i.e. extraction process or long term disposal. These nuclides, C-14, H-3, Kr-85 and I-129, share a similar property in their rather long half-life. If the voloxidation process is employed, semi-volatile materials, such as Cs, Tc, Mo, and Ru, could also be released as part of the off-gas. In general off-gas produced in a nuclear facility must be treated, and the activities of the released gaseous effluent must be below regulatory limits. In IWMS, off-gas treatment concept was designed to accommodate the treatment of the semi-volatile species as well as the volatile ones. The following sections discuss the treatment methodology of each problematic off-gas mentioned.

2.1.4.1 Treatment of H-3

Tritium (H-3 or T) is formed inside irradiated nuclear fuel by fission or neutron bombardment of light elements such as boron or lithium. During the course of irradiation, H-3 is distributed in both the fuel elements and cladding after small leaks during the operation. The amount of H-3 available for release is the portion that remains in the fuel because once it bonds with cladding material which is mostly metal, it is unlikely to transform into gaseous form even during nitric acid dissolution or voloxidation. The H-3 portion that is available for release is a function of operating parameters such as fuel burnup, and is not well determined. In this research, all H-3 estimated by the fuel depletion code was assumed to be in mobilized form. Treatment of H-3 from off-gas is common in nuclear facilities, and is a mature process. It is a similar process to heavy water production, which was commercially employed in countries such as Canada and India. Examples of the methodology used to treat H-3 are: direct storage, isotopic enrichment, distillation, electrolysis, vapor-phase catalytic exchange, liquid-phase catalytic exchange and combined electrolysis and catalytic exchange (CECE)[39]. In this research, CECE was used as a basis of H-3 treatment. The CECE process utilizing wetproofed catalyst is considered the process for extracting tritium from water with high separation factors [40]. This work demonstrated industrial scale heavy water detritiation process with high separation factors.

2.1.4.2 Treatment of C-14

Several treatment methodologies of C-14 are well developed, such as aqueous caustic absorption, fluorocarbon absorption and solid absorption [39]. Because C-14 has a very long half-life, its final waste form must ensure very high integrity for a long period of time to help guarantee a projected dose limit for both humans and the environment in the future. At the present time, the final disposal form has yet been determined. The C-14 from the reprocessing operations is expected to be in the form of CO_2 and is mainly involved in DOG if voloxidation is not utilized. The most common and well developed process is two-step soda scrubbing, i.e. NaOH scrub followed by $Ca(OH)_2$ mixing;

$$CO_2(g) + 2NaOH(aq) \rightarrow Na_2CO_3(aq) + 2H_2O(aq)$$

$$Na_2CO_3(aq) + Ca(OH)_2\,(aq) \rightarrow CaCO_3(s) + 2NaOH(aq).$$

One condition for this process is it must be followed by a NO_x removal process. The final product is a precipitated calcium carbonate which is considered one of the most stable forms of carbon. In the current work, the soda scrubbing technology was assumed. The process parameters required by the IWMS modeling were obtained from [39].

2.1.4.3 Treatment of I-129

Iodine-129 is one of several radioactive iodine isotopes formed as a fission product in irradiated nuclear fuel. Its relatively long half-life of 15.7×10^6 years (other iodine isotopes have quite a short half-life) requires it to be properly managed before permanent disposal. Two major treatment methods, wet scrubbing and solid adsorbents, have been developed to treat radioiodine. Wet scrubbing technique includes alkaline scrub, mercurex process, iodox process, electrolytic scrubbing, fluorocarbon solvents, silicon-organic (polymethylsiloxane) solvents and molten hydroxide [41]. The solid adsorbent method includes activated carbon, macroreticular resins, and silver-based adsorbents such as silver nitrate impregnated substrates and silver zeolites [41]. Some of these methods have been demonstrated in an industrial scale including the silver impregnated silica based method that was used in WAK plant, in Karlsrule, Germany with reasonable decontamination factor [39]. In IWMS modeling, the silver impregnated silica based was used as a baseline for I-129 treatment.

2.1.4.4 *Treatment of Krypton-85 (Kr-85)*

Kr-85 (half-life: 10.76 years) is a direct fission product. Although a small fraction of the Kr-85 leaks from failed fuel elements during irradiation, a majority of it is retained until the fuel elements are chopped and dissolved during reprocessing. It is completely released via DOG if voloxidation is not employed. In the past, there was no regulation on the Kr-85 gas release which means it was released to the environment. However, a new set of rules now require that Kr-85 must be retained and regulated in a safe manner. Although a number of processes have been proposed for the removal of Kr-85, including cryogenic distillation, fluorocarbon absorption, adsorption, diffusion and selective membrane processes, these treatment methods have not been implemented in the nuclear industrial scale. Among the methodologies mentioned, cryogenic distillation received the most attention by most countries because the technology is a well-proven one used in the air products industry. It can be readily adapted to commercial Kr-85 removal but needs some further development to adjust it to the special conditions and problems of the nuclear industry. As result, this technique was used in the IWMS modeling [42].

2.1.5 Reprocessing scheme

The IWMS reprocessing scheme can be constructed by combining previously explained processes, i.e. the head-end process, the separation process and the support process. The UREX process was a baseline process for IWMS modeling. Table 2-2 gives an example of possible process variations of UREX+ process.

Table 2-2 UREX+ process and its possible variations

Process	1st Product	2nd Product	3rd Product	4th Product	5th Product	6th Product
UREX+1	UREX		CCD-PEG/FPEX	TRUEX/TALSPEAK		
	U	Tc	Cs/Sr	TRU+LN	FPs	
UREX+1a	UREX		CCD-PEG/FPEX	TRUEX/TALSPEAK		
	U	Tc	Cs/Sr	TRU	Ac/Ln	FPs
UREX+2	COEX			CCD-PEG/FPEX	TRUEX/TALSPEAK	
	U	Tc	Np+Pu	Cs/Sr	Am+Cm+LN	FPs
Case study	UREX		FPEX			
	U	Tc	Cs/Sr	FPs		

2.2 Radioactive Waste Classification

2.2.1 International Atomic Energy Agency (IAEA) Waste classification

The IAEA approach categorizes six classes of radioactive waste as follows [43]:

2.2.1.1 **Exempt waste (EW)***:*

EW is the waste that meets the criteria for clearance, exemption or exclusion from regulatory control for radiation protection purposes as described in Reference [44].

2.2.1.2 Very short lived waste (VSLW):

VSLW is the waste that can be stored for decay over a limited period of up to a few years and subsequently cleared from regulatory control according to arrangements approved by the regulatory body, for uncontrolled disposal, use or discharge. This class includes waste primarily containing radionuclides with very short half-lives often used for research and medical purposes [43].

2.2.1.3 Very low level waste (VLLW):

VLLW is the waste that does not necessarily meet the criteria of EW, but that does not need a high level of containment and isolation and, therefore, is suitable for disposal in near surface landfill type facilities with limited regulatory control. Such landfill type facilities may also contain other hazardous waste. Typical waste in this class includes soil and rubble with low levels of activity concentration. Concentrations of longer lived radionuclides in VLLW are generally very limited [43].

2.2.1.4 Low level waste (LLW):

LLW is the waste that is above clearance levels, but with limited amounts of long lived radionuclides. Such waste requires robust isolation and containment for periods of up to a few hundred years and is suitable for disposal in engineered near surface facilities. This class covers a very broad range of waste. LLW may include short lived radionuclides at higher levels of activity concentration, and also long lived radionuclides, but only at relatively low levels of activity concentration [43].

2.2.1.5 Intermediate level waste (ILW):

ILW is the waste that, because of its content, particularly of long lived radionuclides, requires a greater degree of containment and isolation than that provided by near surface disposal. However, ILW needs no provision, or only limited provision, for heat dissipation during its storage and disposal. ILW may contain long lived radionuclides, in particular, alpha emitting radionuclides that will not decay to a level of activity concentration acceptable for near surface disposal during the time for which institutional controls can be relied upon. Therefore, waste in this class requires disposal at greater depths, of the order of tens of metres to a few hundred metres[43].

2.2.1.6 High level waste (HLW):

HLW is the waste with levels of activity concentration high enough to generate significant quantities of heat by the radioactive decay process or waste with large amounts of long lived radionuclides that needs to be considered in the design of a disposal facility for such waste. Disposal in deep, stable geological formations usually several hundred metres or more below the surface is the generally recognized option for disposal of HLW[43].

A summary of the IAEA waste classification is also shown in Table 2-3.

Table 2-3 Radioactive waste classifications and possible disposal options

		Long-lived	Short-lived	Very short-lived (VSLW)
	Period Activity	> 30 years	≤ 30 years > 100 days	≤ 100 days
High Level (HLW)	$> 10^{8}$ Bq/g	Deep geologic repository		Decay storage
Intermediate Level (ILW)	$\leq 10^{8}$ Bq/g $> 10^{5}$ Bq/g	Deep geologic repository	Near-surface disposal	
Low Level (LLW)	$\leq 10^{5}$ Bq/g $> 10^{2}$ Bq/g	Near-surface disposal		
Very Low Level (VLLW)	$\leq 10^{2}$ Bq/g	Near-surface disposal		

2.2.2 U.S. Waste Classification

All of the U.S. radioactive waste classes, except for the transuranic waste (TRU) and Low Level Waste (LLW), are source-defined, instead of using a common basis, such as a combination of the heat-generation rate and the half-life. The U.S. waste classification system has some classes that share one basis and others that share another. Specific classes were created for sources of waste that are of concern either because of their intense radioactivity (HLW and UF) or because of the immense volume of material (uranium mill tailings). LLW is defined to include any material covered by the Atomic Energy Amendments Act (hereafter the AEA) that does not fit the definitions of the source-defined classes and TRU. Table 2-4, Table 2-5 and Table 2-6 (Taken from [45]) give summaries of the current U.S. radioactive waste definitions.

Table 2-4 Definitions of radioactive waste classes according regulations

Waste Class	Definition
High-Level Waste (HLW)	(A) Highly radioactive materials resulting from the reprocessing of spent nuclear fuel, including liquid waste produced directly in reprocessing and any solid material derived from such liquid waste that contains fission products in sufficient concentrations; and (B) Other highly radioactive materials that the Commission, consistent with existing law, determines by rule and requires permanent isolation[b]. The Commission has determined that irradiated reactor fuel shall, for the purposes of the repository, be considered HLW[c].
Spent Nuclear Fuel (SNF)[d]	Fuel that has been withdrawn from a nuclear reactor following irradiation, the constituent elements of which have not been separated by reprocessing[e]. SNF is regulated as HLW under 10 Code of Federal Regulations (CFR) 60.
Transuranic Waste (TRUW) (Hereafter TRU)	This class is specific to waste streams from Department of Energy (DOE) and comprises "material contaminated with elements that have an atomic number greater than 92, including neptunium, plutonium, americium, and curium, and that are in concentrations greater than 10 nanocuries (nCi) per gram, or in such other concentrations as the Nuclear Regulatory Commission may prescribe to protect the public health and safety."[f] This definition was revised in 1984 by DOE Order 5820.2 to be "Without regard to source or form, waste that is contaminated with alpha-emitting transuranium radionuclides with half-lives greater than 20 years and concentrations greater than 100 nCi/g at the time of assay." (Attachment 2 of Reference[g])
Uranium Mining and Mill Tailings	The tailings or wastes produced by the extraction or concentration of uranium or thorium from any ore processed primarily for its source material content. Also called byproduct materials under 42 United States Code (U.S.C.) § 2014 (e)(2).[h]

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[b] United States Code, Title 42, section 10101 (42 U.S.C. § 10101)

[c] U.S. Code of Federal Regulations, Title 10, Part 60.2 (10 C.F.R. 60.2)

[d] Spent nuclear fuel is the terminology set by regulation. Its physical meaning is similar to used nuclear fuel as used through this dissertation.

[e] U.S. Code of Federal Regulations, Title 10, Part 60.2 (10 C.F.R. 60.2)

[f] United States Code, title 42, section 2014 (42 U.S.C. § 2014)

[g] DOE Order 5820.2 (1984) and replaced by 5820.2A in 1988, both titled "Radioactive Waste Management."

[h] "In the licensing and regulation of byproduct material, as defined in section 2014(e)(2) of this title, or of any activity which results in the production of byproduct material ... a State shall require (1) compliance with the requirements of subsection (b) of section 2113 of this title (respecting ownership of byproduct material and land), and (2) compliance with standards which shall be adopted by the State for the protection of the public health, safety, and the environment from hazards associated with such material which are equivalent ... or more stringent than, standards adopted and enforced by the Commission for the same purpose..."[United States Code, title 42, section 2021 (42 U.S.C. § 2021).].

Table 2-4 Continued

Waste Class	Definition
Low-Level Waste (LLW)	“Radioactive material that (A) is not high-level radioactive waste, spent nuclear fuel, or byproduct material (as defined in[i]); and (B) the Nuclear Regulatory Commission, consistent with existing law and in accordance with paragraph (A), classifies as low-level radioactive waste.”[j] This does not exclude commercial TRU waste. In the government sector, TRU waste is excluded. LLW is divided into two broad categories: waste that qualifies for near-surface burial, and waste that requires deeper disposal. The criteria for near-surface burial are that the external exposure to a member of the public resulting from release of the waste shall not exceed 25 mrem/year, effective dose equivalent; atmospheric releases shall not exceed limits in the National Emission Standards for Hazardous Air Pollutants (NESHAPS[k]); the dose (DOE Order uses “effective dose equivalent,” 10 CFR 61 uses “whole-body dose”) to a person who inadvertently intrudes into the disposal site (under specified scenarios) after loss of institutional control (100 years), shall not exceed a one-time commitment of 5mSv or an annual dose of 1 mSv for first 1000 years after emplacement. LLW that is regulated by the U.S. Nuclear Regulatory Commission (NRC) and qualifies for near surface burial is separated into the three classes described in Table 2-5. DOE LLW is sub-classified according to facility-specific limitations.
Naturally Occurring and Accelerator- produced Radioactive Materials (NORM/NARM)	“Naturally occurring radioactive material and accelerator-produced radioactive material lie outside NRC's regulatory authority and are subject to health and safety regulation by the States and other Federal agencies”[l]. The waste is generally sub-classified as diffuse (less than 2 nCi/g Ra-226 or equivalent) or discrete (greater than 2 nCi/g Ra-226 or equivalent)[m]. They are under review by the U.S. Environmental Protection Agency (EPA) and may be regulated under the Toxic Substance Control Act (TSCA) or Resource Conservation and Recovery Act (RCRA)[n].

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[i] United States Code, title 42, section 2014 (42 U.S.C. § 2014)

[j] United States Code, title 42, section 2021 (42 U.S.C. § 2021)

[k] U.S. Code of Federal Regulations, Title 40, Part 61 (40 C.F.R. 61)

[l] Federal Register: July 21, 1995 (Volume 60, Number 140) Page 37556-37565

[m] Oak Ridge National Laboratory *Integrated Data Base Report—1995: U.S. Spent Fuel and Radioactive Waste Inventories, Projections, and Characteristics*,DOE/RW-006,Rev.12, December 1996.

[n] The League of Women Voters Education Fund, *The Nuclear Waste Primer* 1993 Revised Edition, Lyons & Burford, New York (1993): pp 25-26.

Table 2-5 Subclasses of low-level waste according to the NRC (10 CFR 61)

LLW Waste Class	Definition
Class A	Low levels of radiation and heat, such that no shielding is required to protect occupational workers or public, rule of thumb states that it should decay to acceptable levels within 100 years.
Class B	Has higher concentrations of radioactivity than Class A and requires greater isolation and packaging (and shielding for operations) than Class A waste.
Class C	Requires isolation from the biosphere for 500 years. Must be buried at least 5 m below the surface and must have an engineered barrier (container and grouting).
Greater Than Class C (GTCC LLW)	This is the LLW that does not qualify for near-surface burial. This includes commercial transuranics (TRUs) that have half-lives greater than 5 years and activity greater than 100 nCi/g.

Table 2-6 Definitions of material that qualify waste classifications

Material Designation	Definition
Special Nuclear Material (SNM)	"(1) plutonium, uranium enriched in the isotope 233 or in the isotope 235, and any other material which the Commission, pursuant to the provisions of section 2071 of [title 42 of the U.S.C.], determines to be special nuclear material, but does not include source material; or (2) any material artificially enriched by any of the foregoing, but does not include source material."[o]
Source Material	Material that is essential to the production of special nuclear material.[p] "(1) uranium, thorium, or any other material which is determined by the Commission pursuant to the provisions of section 2091 of [title 42 of the U.S.C.] to be source material; or (2) ores containing one or more of the foregoing materials, in such concentration as the Commission may by regulation determine from time to time."[q]
By-Product Material (11(e) material)	"(1) any radioactive material (except special nuclear material) yielded in or made radioactive by exposure to the radiation incident to the process of producing or utilizing special nuclear material, and (2) the tailings or wastes produced by the extraction or concentration of uranium or thorium from any ore processed primarily for its source material content."[r]
Transuranic Material (TRU)	Material containing or contaminated with elements that have an atomic number greater than 92.

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[o] United States Code, title 42, section 2014 (42 U.S.C. § 2014)

[p] United States Code, title 42, section 2091 (42 U.S.C. § 2091)

[q] United States Code, title 42, section 2014 (42 U.S.C. § 2014)

[r] United States Code, title 42, section 2014 (42 U.S.C. § 2014)

Table 2-6 Continued

Material Designation	Definition
Contact Handled (CH)	Materials or packages with a surface exposure rate less than 200 mR/h may be handled without shielding for radiation workers.
Remote Handled (RH)	Materials or packages with a surface exposure rate greater than 200 mR/h must be handled remotely for protection of radiation workers. Individual sites may have upper limits, as well[s].
Hazardous Waste (Mixed Waste, MW)	Waste that contains both hazardous material, regulated under RCRA by the EPA, and radioactive material, regulated under the AEA and by the NRC or DOE, is called mixed waste. There are high-level mixed wastes, low-level mixed wastes, and TRU mixed wastes (DOE treats all of its TRU waste as mixed waste[t]). EPA has not yet determined whether SNF will be designated as mixed waste.

2.3 Radioactive Waste Management

Radioactive waste management is an integrated system that involves various activities: accumulation, processing, handling, packaging, transportation, storage, disposal, and decontamination and decommissioning [46]. Since waste management activities involve a tremendous amount of information that could not be explained in detail in this document, only relevant activities that are captured and focused in IWMS modeling are discussed. As this research dealt mainly with radioactive waste associated with UF reprocessing; only selected waste activities occurring down stream of the separation process are discussed, i.e. treatment, conditioning and disposal. The reason these three activities are considered in IWMS was the fact that the treatment and conditioning activities is considered the processes that contribute to the final volume of the radioactive waste, while waste disposal indicates the final outcome of the waste management. In general, these waste management activities depend on a number of factors such as waste types, assigned waste class and etc. As described in the previous section, the U.S. classification comprises of wastes classes from

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[s] Carson, P.H., G.D. Pierce, and R.L. Morton "Sources of Waste" *Radioactive Waste Management and the Nuclear Fuel Cycle*, Vol. 14 (1-2), 1990: pp 27-44.

[t] Oak Ridge National Laboratory *Integrated Data Base (IDB) for 1993: U.S. Spent Fuel and Radioactive Waste Inventories, Projections, and Characteristics*, DOE/RW-006, Rev. 9, March 1994.

front-end, back-end and other miscellaneous origin. The relevant wastes for the focus of this research are mostly the back-end originated wastes such HLW, TRU, LLW and MW (which specifically refers to mixed LLW and mixed TRUs). Hence the waste management activities that relate to these waste classes are described in this document.

2.3.1 Radioactive Waste Treatment and Conditioning

2.3.1.1 Radioactive Waste Treatment

Radioactive waste treatment refers to any operations intended to benefit safety and/or economy by changing the characteristics of the waste. Three basic treatment objectives are: volume reduction, removal of radionuclides from the waste and change of composition. Treatment may result in an appropriate waste form [47]. Treatment of radioactive waste depends on the type of an incoming unprocessed waste. Mechanical treatment such as cutting, shredding, compaction, thermal treatment such as incineration and calcinations, chemical and biological treatment such as acid digestion, chemical oxidation, photolysis, and melting and sintering are commonly used as treatment process in nuclear waste treatment. In general, there is no significant difference in treatment procedure for LLW and HLW except remote manipulation in the HLW case.

2.3.1.2 Radioactive Waste Conditioning and Immobilization

Waste conditioning is defined as the operations that produce a waste package suitable for handling, transport, storage and/or disposal. Conditioning may include the conversion of the waste to a solid waste form, enclosure of the waste in containers, and, if necessary, providing an overpack[47]. Conditioning can refer to an immobilization, a conversion of waste into a waste form by solidification, embedding or encapsulation. The aim is to reduce the potential for migration or dispersion of radionuclides during handling, transport, storage and/or disposal[47]. Common matrices used to immobilize the waste are concrete, bitumen, polymer for LLW and borosilicate glass for HLW. These matrices also dictate the final waste form of the conditioning waste.

2.3.2 UF management

Most UFs are currently stored at the utility sites either in wet or dry storage. These types of storage are considered non-permanent. According to the U.S. current policy, once the geologic repository is ready to operate, these UF will be permanently disposed in it under many stringent rules; packaging under interrelated constraints such as maximum mass loading with minimum heat load that also prevent criticality. The research related to these areas has been extensively conducted through these years. Different designs and ideas have been proposed under the current policy. The fundamental objective of UF disposal is to isolate and confine the UF from the environment. With the inherent characteristics of UF, i.e. long-lived radionuclides contents, decay heat generation, and its radiation level, achieving this objective is quite challenging. A Multi-barrier approach was implemented, i.e. the UF must be encapsulated in a canister. The UF canister must be carefully loaded in the repository, followed by backfilling the repository with appropriate material and maintaining monitoring and surveillance thereafter to assure the isolation. Figure 2-1 illustrates the multi-barrier concept implemented in Sweden.

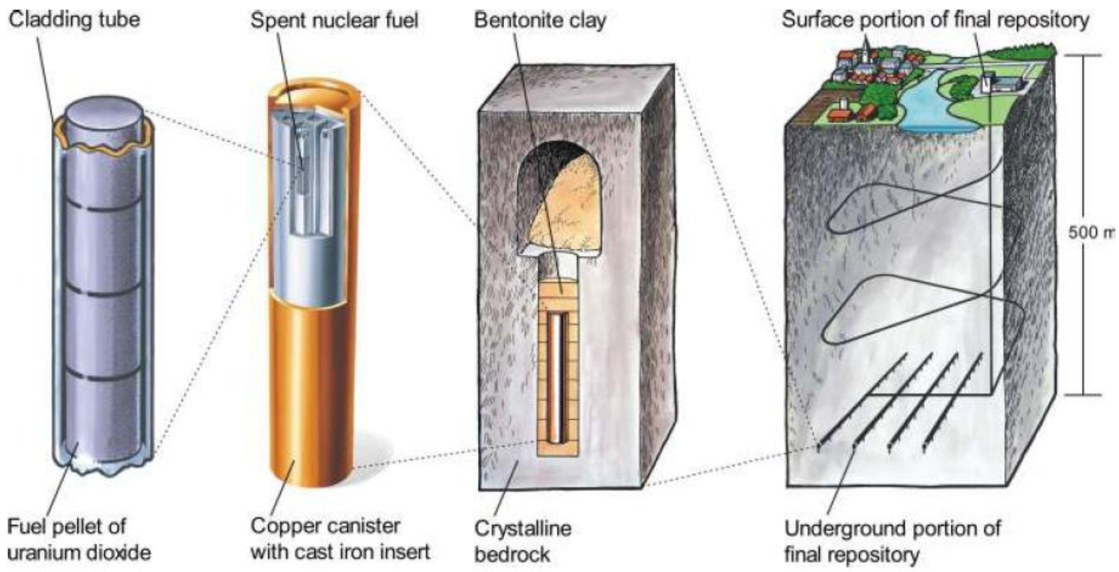

Figure 2-1 The Swedish concept for disposal of UF[u]

2.3.3 Radioactive Waste Disposal

Radioactive waste disposal refers to an emplacement of waste in an appropriate facility without the intention of retrieval. Some countries use the term disposal to include discharges of effluents to the environment [47]. Two common types of radioactive waste disposal are near-surface and geologic disposals. These were the only two types of disposal options used in the IWMS modeling. They are generally designed for low level and high level radioactive wastes respectively.

2.3.3.1 Low level Waste (near surface) Disposal

Near surface repository is a facility for disposal of radioactive waste located at or within a few tens of meters from the earth’s surface [47]. In the U.S., different low level waste disposal facilities accept certain types of low level wastes, i.e. class A, class B or Class C, from certain waste compacts. A compact is defined as a group of nearby states. As of May

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[u] http://www.iaea.org/About/Policy/GC/GC50/GC50InfDocuments/English/gc50inf-3-att5_en.pdf

2010 there are currently 10 compacts, 9 unaffiliated states and the District of Columbia[v]. This radioactive waste disposal is regulated by the U.S. Nuclear Regulatory Commission (NRC). In the case that low level radioactive waste contains a chemically hazard material, the waste is called mixed radioactive waste (MW). Mixed waste is regulated by both the NRC and the U.S. Environmental Protection Agency (EPA). If it meets the acceptance criteria, it can be disposed of in the Land Disposal Restriction (LDR) facility, the same as chemical and toxic wastes. At present, Waste Control Specialists LLC in Andrews County, Texas[w], has applied for a license for the near surface disposal of LLW. If the facility is granted the license, it will accept mixed low level radioactive waste (MLLW) (only class A) from around the country.

2.3.3.2 High Level Waste (geologic) Disposal

A geological repository is a facility for disposal of radioactive waste located underground (usually several hundred meters or more below the surface) in a geological formation to provide long term isolation of radionuclides from the biosphere[47]. It is commonly used to store high level radioactive waste or UF. The only designated facility for the geologic repository is the Yucca Mountain Facility (YMF). However, the YMF has not been granted a license, hence, in practice, there is currently no geological repository for HLW and UF.

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[v] http://www.nrc.gov/waste/llw-disposal/licensing/compacts.html

[w] http://www.urs-slc.com/wcs/

Chapter 3 Integrated Waste Management Model Development

To achieve the goal for this research, a computer code named Integrated Waste Management Simulation (IWMS) was developed. The code has two major components; a main IWMS calculation unit which was written in FORTRAN [48], and a main user-interface unit done in a Microsoft Excel spreadsheet. For deterministic calculation, user-defined parameters are generated on the fly into a series of text files using Visual Basic (VB) embedded in Microsoft Excel. Although most of the calculations take place in the FORTRAN unit, there is one specific calculation that automatically utilized MATLAB software [49], i.e. the user-specified weights for decision making analysis. Next, these text files are imported to the main IWMS FORTRAN code for the corresponding calculation. Text output files are simultaneously created. Because these files contain too much information and revealing all of the information in these files is not necessary, only some of the major results are imported back into different MS Excel spreadsheets for easier interpretation and analysis. For probabilistic calculation, @Risk software [50], a MS Excel based software, was utilized to achieve the task. @Risk allows users to specify a probability distribution for any uncertain user-input parameter. Together with the help of VB in MS Excel, an executable IWMS file (the main calculation unit of the IWMS code) can be called from MS Excel. @Risk software changes the input parameter according to a previously assigned probability distribution. After each input parameter changes, the main IWMS calculation unit is run, each set of output parameters is created and imported back to MS Excel. @Risk collects each set of output parameters after each input changes. These steps are repeated many times (or simulations) until the goal (usually a maximum number of iteration) is reached. Once the whole calculation is completed, @Risk performs the necessary post-processing of the output data.

General IWMS code features include: (1) an advanced aqueous separation calculation capability that can define and estimate the amount and inherent properties of all product streams associated with all user specified UF aqueous separation processes such as UREX, UREX+1, or COEX, refabrication and supported processes (a unique combination of user-defined process is called reprocessing scheme in this research); (2) a scheme to preselect a qualified management option(s) (decay storage follow by disposal, decontamination then reuse, and transmutation) that could be economically applied to each of the product streams derived from the previous step, with direct disposal as a defaulted alternative; (3) decision making models on a waste management alternative based on the preselected options from the previous step and on waste form materials for the defaulted direct disposal alternative; (4) parameters acquisition modules to calculate the required parameters for supporting the two decision making levels and; (5) calculation results summary. Please note that steps 3 and 4 are repeated for each derived stream arisen according to a user-specified reprocessing scheme. Figure 3-1 illustrates the conceptual flow of these tasks. Details of these features are also described in the following sections.

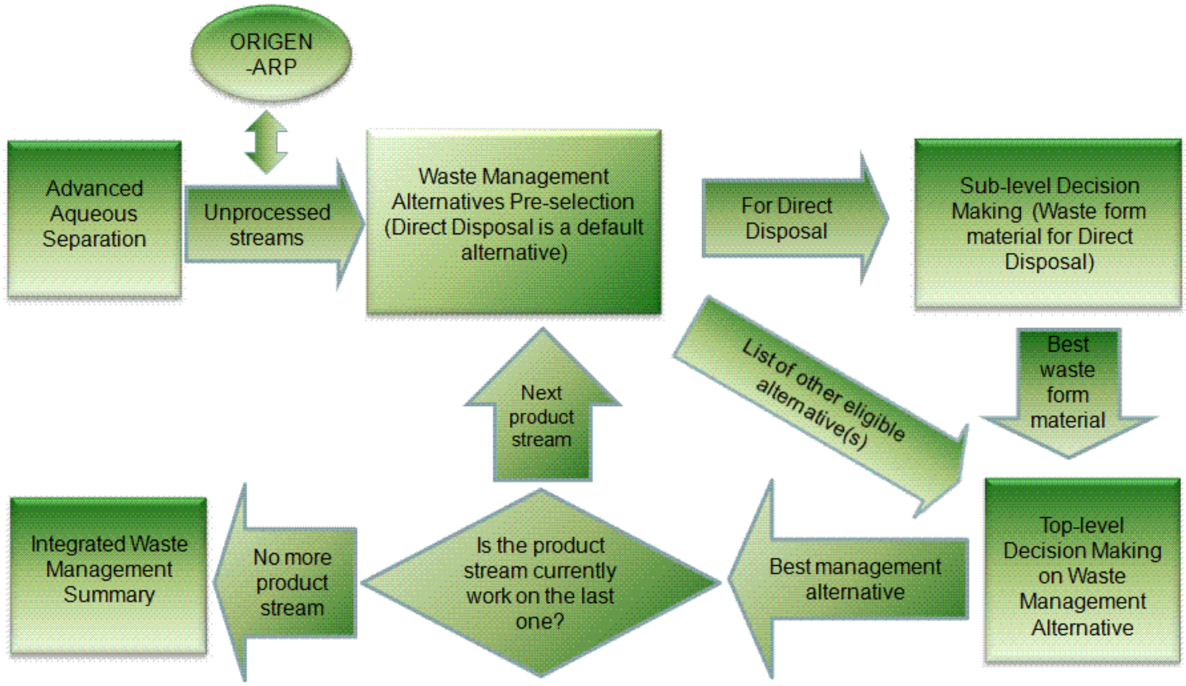

Figure 3-1 Simplified IWMS work flow model

3.1 Advanced Aqueous Separation Process Calculation

3.1.1 UF Reprocessing and Flow through the IWMS

Reprocessing usually starts by disassembling UF assemblies. This process aims at de-structuring the fuel assemblies into fuel rods and structure materials. While the fuel rods are passed through the head-end of the reprocessing process, the activated structure materials are sent to the next step of the process. Once the fuel rods are separated during chopping process, they are cut into small pieces in order to improve their dissolution in the later step. Next, chopped fuels are either advanced directly to the fuel dissolution or voloxidized to get fuel powder prior to the fuel dissolution. All fission gas is assumed to release during these stages and is rerouted to the off-gas treatment system. The fuel solution is then passed on to the separation process. UREX is chosen in order to be consistent with the current national separation baseline process. The UREX process extracts uranium and technetium and leaves behind the rest of the fission products in its raffinate which will be further extracted in the next separation process if other elements are to be further separated. Uranium, the main product from UREX, is forwarded to the conversion and refabrication processes and remanufactured to MOX fuel which will be put back into the light water reactor. Technetium (Tc) is kept separately in the storage facility for treatment decision, i.e. transmutation and then permanent disposal, reuse, or direct disposal. Depending on the desired reprocessing scheme, UREX raffinate can be fed to the next step of the separation process in the advance separation scheme, typically the Cesium (Cs) and Strontium (Sr) separation process (due to their contributions to short term heat generation); or directed to a vitrification process to produce final waste forms for permanent disposal. Either FPEX or CCD-PEG process can be used to retrieve Cs and Sr. Once Cs and Sr are separated, they await management decision. Depend on whether further elements retrieval is needed, the raffinate from Cs/Sr separation process is either forwarded to TRUEX, with small solution adjustment, or directed to a vitrification process to produce final waste forms for permanent disposal. TRUEX separates both actinides and lanthanide from the main raffinate stream and the rest of fission products remain in TRUEX raffinate for further treatments. Since the current policy requires no further separation of another element from this particular TRUEX raffinate, it will be directed to a vitrification process to produce final the waste forms for permanent disposal. The UREX+ baseline process is designed to separate the actinides and lanthanides from the TRUEX product stream described earlier. To achieve this task, either TALSPEAK or Reversed TALSPEAK can be employed to extract actinides from lanthanides. As results, actinides and lanthanides are to be kept in separate streams. While Lanthanides are subjected to a treatment decision in the same way as Tc and Cs/Sr, actinides can be used as a next generation nuclear fuel after being routed to the next generation fuel fabrication process.

3.1.2 Process and Stream Definitions

Unlike the typical separation process that usually does not include fuel refabrication, the IWMS code constitutes fuel refabrication as part of its scheme for a comprehensive analysis of the entire back-end process. The IWMS scheme accounts for head-end, aqueous separation (so called solvent extraction), refabrication, and supported processes as shown in Figure 1-5. From this figure, the 4 diamond boxes show that users can alter the reprocessing scheme as desired which makes at least 16 different reprocessing schemes that could be evaluated. Different schemes generally result in different numbers of derived products streams. The physical processes, aqueous separation, fuel refabrication, or support process, are designated by rectangular boxes. Each box has a unique name that corresponds to its physical meaning, for example, DISB refers to fuel disassembling, CHOP refers to fuel chopping or shredding, VOLX refers to voloxidation, UREX refers to URanium EXtraction and etc. Each process, or box, has defaulted incoming (raw material or RM) and outgoing (product or P) streams which can be categorized into 2 types, i.e. Type I (T1) and Type II (T2) which refer to any stream that has an origin from (in case of incoming stream) or a destination to (in case of outgoing stream) another process within the reprocessing scheme. In IWMS, all incoming and outgoing streams were predefined for a particular process. Table 3-1 gives a summary of predefined number of all stream types.

Table 3-1 Summary of process descriptions

Process code	Process Name	Subroutine Name	Number of predefined stream (s)			
			Type 1 Incoming stream	Type 2 Incoming stream	Type 1 Outgoing stream	Type 2 Outgoing stream
DISB	Disassembling	DISB_BOX	0	1	1	1
CHOP	Chopping	CHOP_BOX	1	0	2	1
VOLX	Voloxidation	VOLX_BOX	1	0	2	1
DISS	Dissolution	DISSV_BOX[x]	1	1	1	0
		DISSC_BOX[y]	1	1	2	2
UREX	UREX	UREX_BOX	1	7	2	3
COEX	Co-Extraction	COEX_BOX	1	11	2	4
FPEX	FPEX[z]	FPEX_BOX	1	8	1	3

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[x] Dissolution with voloxidation

[y] Dissolution without voloxidation

[z] Fission Product Extraction process

Table 3-1 Continued

Process code	Process Name	Subroutine Name	Number of predefined stream (s)			
			Type 1 Incoming stream	Type 2 Incoming stream	Type 1 Outgoing stream	Type 2 Outgoing stream
CCDPEG	CCDPEG[aa]	CCDPEG_BOX	1	8	1	3
TRUEX	TRUEX[bb]	TRUEX_BOX	1	11	1	4
TALSPEAK	TALSPEAK[cc]	TALSPEAK_BOX	1	8	1	4
REVTAL	Reversed TALSPEAK	REVTAL_BOX	1	7	1	4
MOXFUEL	Conversion & MOX fuel Fabrication	MOXFUEL_BOX	1	2	0	2
NEXFUEL	Conversion & Next general fuel fabrication	NEXFUEL_BOX	1	2	0	1
OFGT	Off-gas Treatment	OFGTV_BOX	2	7	0	7
		OFGTC_BOX	2	4	0	4

To give an example of how IWMS defined streams in general, the chopping process receives used fuel rods from dissembling process and produces chopped fuel rods, fission gas and small scraps. First, for the disassembling standpoint, which is the required process prior to fuel chopping, the fuel rods stream was defined as DISBT1P1. Second, for the chopping process standpoint, this fuel rods stream was also defined as CHOPT1RM1 and after chopping, chopped fuel rod or fuel hull was defined as CHOPT1P1; fission gas released during fuel chopping was defined as CHOPT1P2; and the scraps were defined as CHOPT2P1 because metal scraps would be subjected to one of the management strategies. Besides these direct streams from the process, secondary waste streams were also considered in IWMS. Because these secondary waste streams are usually small in radioactivity but vary in material types, they were not categorized in the same way as the direct streams. Instead 12 different types of secondary waste were defined, and unique codes were used, i.e. CHOPfilter,

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[aa] Chlorinated Cobalt Dicarbollide Poly Ethylene Glycol

[bb] Transuranic Extraction

[cc] Trivalent Actinide Lanthanide Separation by Phosphorus reagent Extraction from Aqueous Komplexes

CHOPEquip, and etc. A completed list of direct incoming and outgoing streams and their descriptions; and secondary waste streams are given in Appendix A and B, respectively. To illustrate the process, Figure 3-2 and Figure 3-3 show the details of disassembling and chopping processes and their flows. The flow diagrams of other processes employed in IWMS are given in Appendix C.

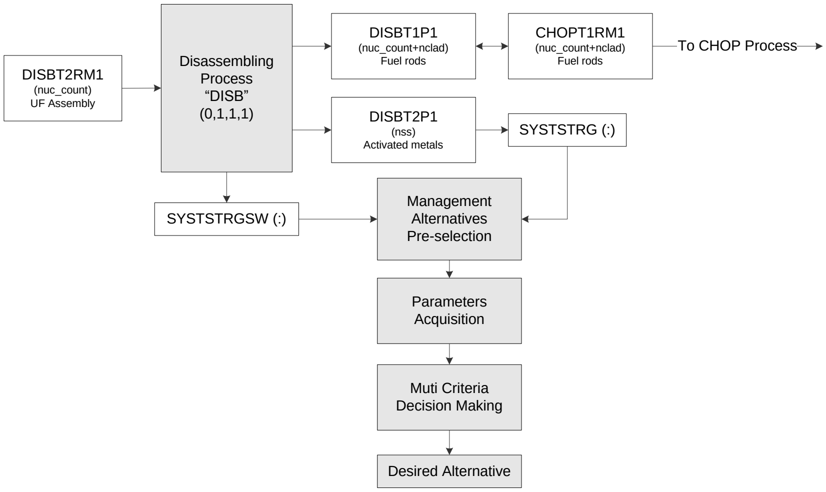

Figure 3-2 Disassembling process flow diagram

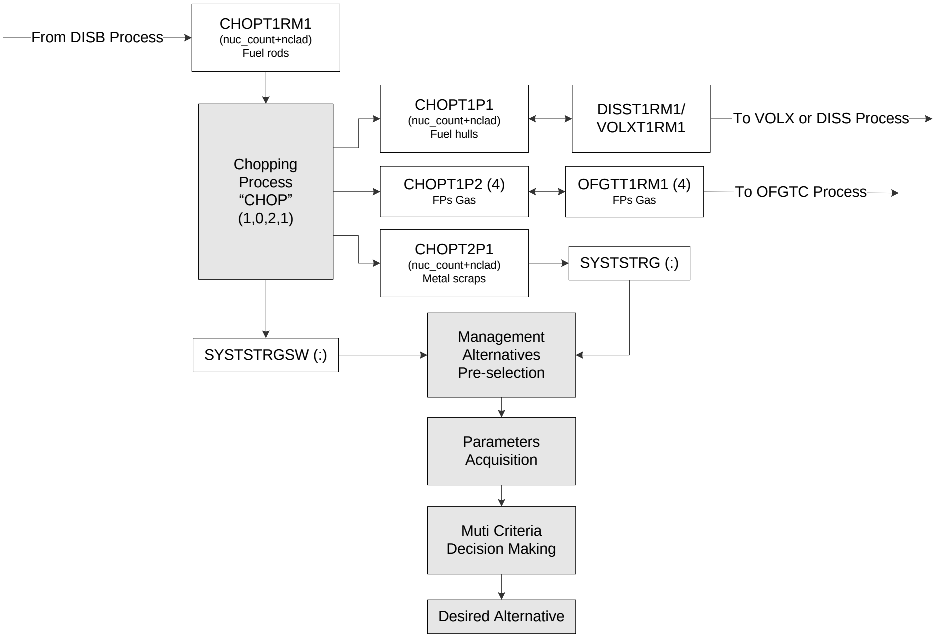

Figure 3-3 Chopping process flow diagram

3.1.3 Materials Balance Calculation

To calculate materials distributed among incoming and outgoing streams under limited resources, various assumptions were made, including 1) mass conservation for both the entire reprocessing scheme and individual processes; 2) no neutron multiplication; 3) radioactivity conservation, i.e. no radiological decays during fuel separation; 4) target separation efficiency based calculation, i.e. the mass of interested material in the designate product stream is calculated based on target separation efficiency and, 5) steady state condition for all aqueous separation processes. To illustrate the mass balance concept, the UREX process (Figure 3-4) is chosen for demonstration. The mass of various radionuclides distributed across UREX process can be calculated based on the previously described assumptions and predefined UREX flow diagram. Figure 3-4 also shows how the mass and the activity of the radionuclides of interest for UREX process can be determined.

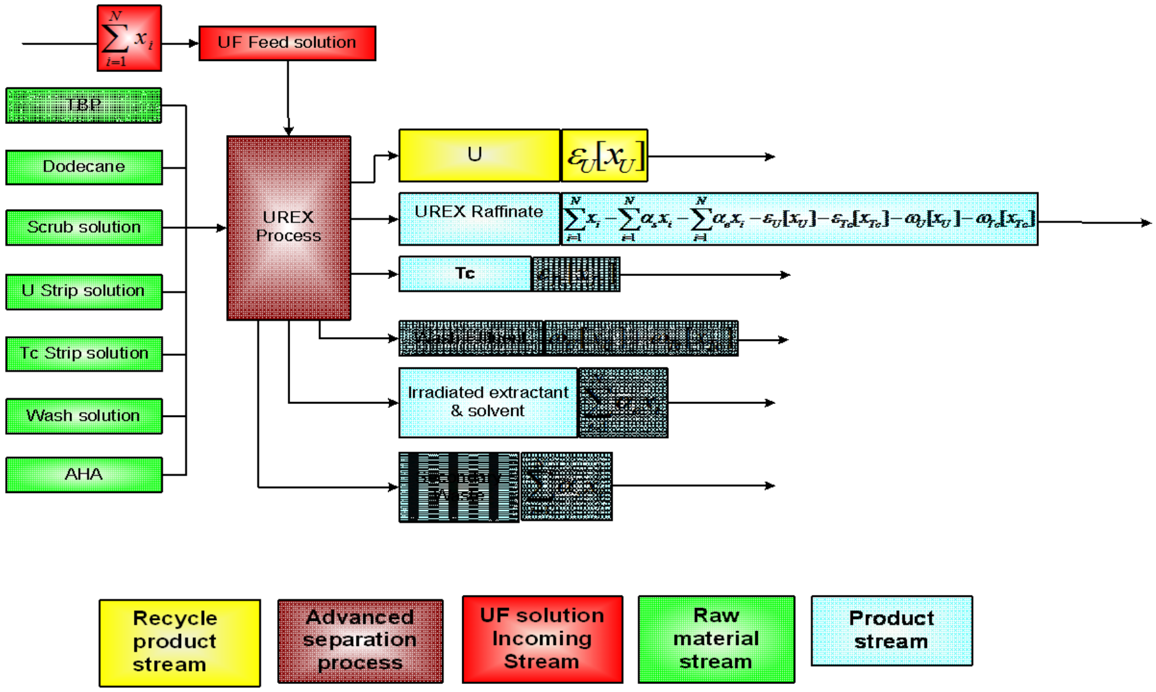

Figure 3-4 UREX process flow diagram and material distributions

where x_i is a mass (kg) or activity (Bq) of element i; ε_i is a target separation efficiency of element n; ω_i is a fraction of element i distributed in wash effluent; α_e is a fraction of relevant elements distributed in spent solvent (this value was assumed to be the same for all relevant elements, and zero for all non-relevant elements) and α_s is a fraction of all the elements distributed in secondary waste streams (this value was also assumed to be the same for all elements). Since the separation process is a chemical process, different isotopes of the same elements are treated essentially the same way for a given chemical separation process. This approach was applied to all the processes employed in IWMS.

From Figure 3-4, raw material streams are represented by green and categorized by type II incoming (raw material) stream. Initial UF solution feed is indicated by red and categorized by type I incoming stream. Yellow shows the product (outgoing) stream of type I. Blue denotes both of the type II product streams and secondary waste streams. In summary, the UREX process consists of;

- 1 stream of Type I input—continuing stream from UF dissolution
- 7 streams of Type II input—raw materials for the UREX process
- 2 streams of Type I output —U stream (which proceeds to MOX fuel fabrication) and UREX raffinate (which proceeds to either FPEX/CCDPEG or vitrification)
- 3 streams of Type II output—Tc stream, wash effluent and spent solvent
- Secondary waste streams

To quantify the materials distributed in all of the product streams from the process and their volumes, the following parameters are required: (1) radionuclides inventories in all relevant incoming streams, (2) steady state volumetric flow rate of all incoming streams, i.e. both type I and II raw material streams; (3) steady state volume and radioactivity contributions of all relevant secondary streams; (4) target separation efficiency if the relevant process is an aqueous separation process; (5) elemental dissolution efficiency in nitric acid; and (6) fission gas release fraction in the head-end process. Since IWMS takes into account the cost as one of the decision criteria for waste management options (details are described later in this chapter), unit costs data are also required. These parameters are needed for all the processes (i.e. head-end, separation and supported processes) employed in IWMS modeling. They were used as part of IWMS input parameters. Other IWMS input parameters are described later as needed.

3.2 Derived (Waste/Non-Waste) Stream Management Alternatives and Pre-selection Criteria

As the calculations proceed, product streams are automatically created based on the user-defined reprocessing scheme and other given input parameters. Once all of the derived streams are completely defined, IWMS considers the inherent properties of each derived stream in order to predetermine eligible management alternative(s) for making decisions on the best management strategy for that particular stream. To save calculation resources, the alternative(s) pre-selection process was designed to pre-select the qualified waste management alternative for a given incoming waste stream because only certain waste streams are qualified for all available alternatives in this research. Two levels of decision making were incorporated in this research.

3.2.1 IWMS Top-Level Decision Making

The top-level decision making relates to the waste stream management alternative. These decisions are to be made among five alternatives: (1) direct disposal; (2) decay and storage follow by near surface disposal; (3) transmutation follow by disposal; (4) decontamination and recycle follow by disposal non-usable part; and (5) exempt. Except for the direct disposal that always serves as a defaulted alternative, the rest of the alternatives are pre-selected based on the requirements written in the scheme shown in Figure 3-5. Details on how the alternative(s) are selected are explained in the following section. Once the eligible alternative(s) has been determined, the best alternative will be chosen against three criteria, alternative costs, the Committed Effective Dose Equivalent (CEDE) and the feasibility of the alternative technology.

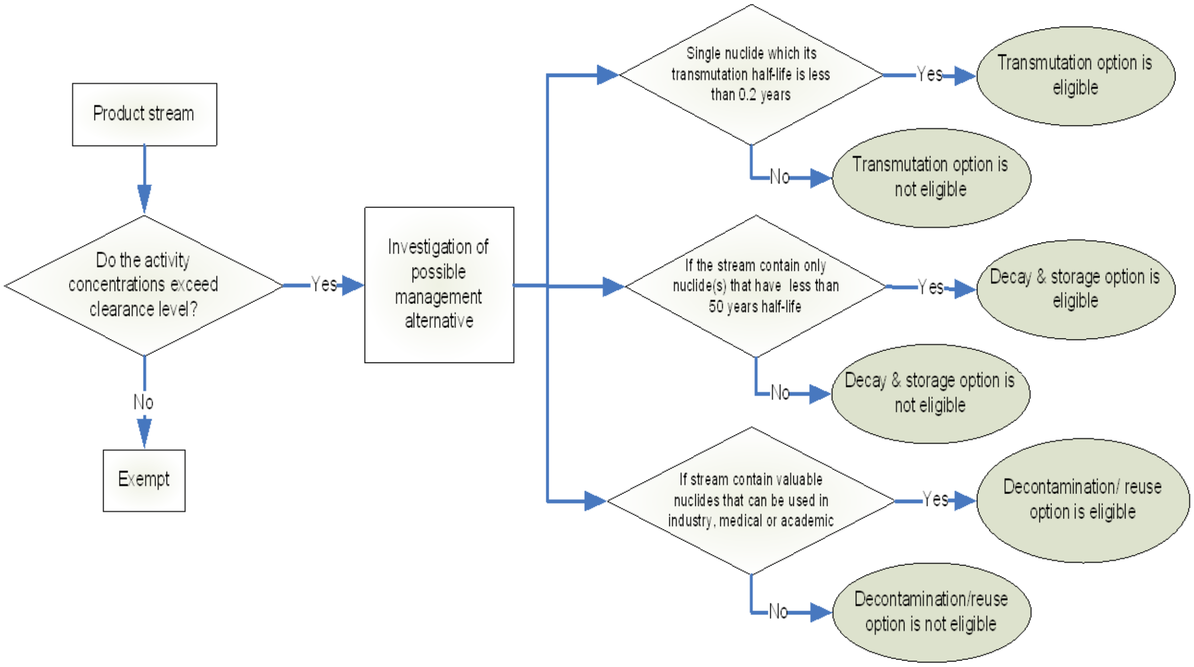

Figure 3-5 Management alternative pre-selection scheme

3.2.1.1 Exempt Option

The first requirement is to differentiate the stream to be discarded (exempted) based on the clearance radionuclides concentrations level set by the International Atomic Energy Agency (IAEA)[44 ,51]. A summary of the concentration limits for each radionuclides is given in Appendix H. Basically, if radionuclides concentrations in a particular stream have not exceeded these clearance concentrations level, such a stream can be released without any treatment. If the stream cannot be unconditionally released, it proceeds to the next requirement checkpoint. At this check point, logical conditions (true or false) are evaluated.

3.2.1.2 *Decay Storage Option*

The conditions for the decay and storage alternative include existence of radionuclide with a half-life of 50 years or less. These radionuclides are all Cesium (Cs) isotopes, (Cs-134, Cs-134m, Cs-135, Cs-136, Cs-137, Cs-140, Cs-141, Cs-142, Cs-143, Cs-144, Cs-145, Cs-14) and most Strontium (Sr) isotopes (Sr-87m, Sr-89, Sr-90, Sr-91, Sr-93, Sr-95, Sr-99 and Sr-103). After a storage time of 150 years, radionuclides inventories are updated using ORIGEN output at that time. Based on these updated inventories, only LLW treatment, conditioning and disposal are assumed. Current technology and cost data for all processes mentioned were applied in the current IWMS model, since future data is simply not available. For storage cost, dry UF storage nominal cost of 120 USD/kgU [52] was used, since individual storage of these radionuclides is not available.

3.2.1.3 *Transmutation Option*

The conditions for transmutation include (1) existence of only one radionuclide in the stream, (2) having such radionuclide as a member of the transmutation database and (3) developing less than 0.2 years transmutation half-life. Evaluation of transmutation half-life is given later in this chapter. The radionuclides that are eligible for transmutation are: I-129, Tc-99, Np-237, Am-241, Am-243, Cm-245, Cm-246, Cm-247, Cm-248 and Cm-250. Transmutation devices (neutron production devices) considered in IWMS are: Deuterium-Deuterium (D-D) reactions based device, Deuterium-Tritium (D-T) reactions based device and D-D reactions with un-moderated neutron [53]. To qualify for the transmutation option, the effective transmutation half-life must be greater than 0.2 years (in one or more of the transmutation systems mentioned). The effective transmutation half-life (τ_{eff}) can be calculated by:

$$\boldsymbol{\tau_{eff}(y) = \frac{ln\,(2)}{3.1557*10^{7}*\sigma(E)*\phi(E)*f_n}} \qquad \textbf{Equation 3-1}$$

where σ is the neutron absorption (fission and capture) cross sections ($\frac{cm^2}{\mathrm{n}}$), ϕ is the neutron flux $\left(\frac{n}{sec-cm^2}\right)$ and f_n is neutron utilization efficiency (0.5 was used [54]). Since both neutron cross section and neutron flux are energy dependent parameters, to determine the transmutation half-life, the collapsed one energy group average approach was used. Neutron fluxes as a function of energy for all devices were obtained from Sit, Roger [53]. Neutron absorption cross sections were collected from Evaluated Nuclear Data File (ENDF) Database, software version of May 31, 2010[dd].

3.2.1.4 Decontamination and Recycle Option

The conditions for decontamination and recycle include (1) having radionuclide (s) as a member of recycling database and (2) providing an overall benefit, i.e. economically separation of such radionuclide(s) with an industrial, medical or academic application. Radionuclides in the recycling database include C-14, Ce-144, Eu-149, Eu-150, Eu-154, Eu-155, Eu-156, H-3, Ho-166m, Kr-85, Pm-146, Pm-147, Sm-145, Sm-146, Sm-148, Sm-151 and Sm-155. Currently, a few of these radionuclides have significant applications, hence market values and separation costs for most of these radionuclides were assumed. This database could be updated once more accurate information is available.

3.2.1.5 Direct Disposal Option

The direct disposal option is a defaulted alternative in the IWMS code. Under this option, the preferred waste form material will be selected via the sub-level decision making process described in the following section. To proceed with the calculation, assumptions on the disposal site were made. Two disposal facilities were assumed: direct disposal in Land Disposal Restriction (LDR) Site and direct disposal in a geologic repository. Near-surface land disposal of low-level radioactive waste in Andrews County, Texas was used as a representative site for Low Level radioactive Wastes (LLW) and Mixed Low Level Wastes (MLLW) disposals. All relevant information required in the calculations such as groundwater transport calculations for LLW, were obtained from this site. The Yucca Mountain disposal

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[dd] http://www-nds.iaea.org/exfor/endf.htm

facility was used as a representative site for High Level Wastes (HLW) and commercial TRansUranic wastes (TRU) disposals. All relevant information required in the calculations, such as groundwater transport calculations for HLW, was obtained from the Yucca Mountain site.

3.2.2 IWMS Sub-Level Decision Making

The sub-level decision making is made under the direct disposal option. This decision making is to choose the waste form material; i.e. borosilicate glass, ceramics, or metal if as-generated waste is HLW, TRU or MTRU; and concrete, polymer or metal if generated waste is LLW or MLLW. Decision criteria include (1) waste form development cost (2) CEDE at the disposal site boundary at 10000 years after permanent disposal (3) intruder dose (radiation dose to an intruder) at the disposal facility (4) worker exposure dose at the waste processing facility and (5) compatibility between the proposed waste form material and waste stream properties.

3.3 Decision Making Methodology

Making decisions in waste management alternatives is a complex process, involving multiple attributes. Attributes are also referred to as “goals” or “decision criteria”. Attributes represent the different dimensions from which alternatives can be viewed. Alternatives usually represent the different choices of action available to the decision maker.

The described decision criteria have different units, or sometimes no units. Examples are: total volume of conditioned waste forms, total costs, total radiation doses, and the feasibility of the technology employed. To take into account this difference and to be able to efficiently compare management alternatives, a method such as Multi Criteria Decision Analysis (MCDA) [55] is needed. MCDA is one of the most well known branches of decision making, and has been extensively researched and applied to many types of problems. It generally serves as a decision making tool for a decision maker. Several components for MCDA such as alternatives, decision criteria are explained in the previous section except for the decision weight and the decision matrix. In this research, Weighted Product Model (WPM), one of the MCDA tools, was used as a decision making tool.

3.3.1 Decision weights

The MCDA method requires that criteria be assigned weights of importance. They indicate priorities or how significant the decision criterion is relative to each of the others. These weights normally add up to one. To determine the decision weight, the Analytical Hierarchical Process (AHP) [56] weight derivation method was used. This weight derivation process starts by making a pairwise comparison matrix of each decision criteria by first assigning the relative degree of dominance to each pair. (For example, if one criteria is "absolutely dominant" over the other, the dominant criteria would be given the value 9, the other the reciprocal value). Next construct a matrix out of the pairwise values. It will have 1's on the diagonal and will have a reciprocal of each term reflected across the diagonal. Next find the real eigenvector of the matrix and the corresponded real eigenvector. The numbers in the eigenvector represent the relative importance of the criteria. These numbers were normalized to make the weight vector, i.e. the sum of all elements in the weight vector sum up to unity. Weight can be automatically calculated from user-specified relative importance between decision criteria described earlier in this section through the MS excel spreadsheet named “top_level” and “sub_level” for top-level and sub-level decision making respectively. If not specified by the user, defaulted weights (based on expert judgment which is subjective to a specific case study and should be implemented with careful consideration) will be used in the calculations.

3.3.2 Decision Matrix

A MCDA problem can be written in matrix format (Figure 3-6). A decision matrix A is an m-by-n matrix in which element a_{ij} indicates the performance of alternative A_i when it is evaluated in terms of decision criterion C_j (for $i = 1,2, \dots, m$ and $j = 1,2, \dots, n$)[55]; i.e.

$$\begin{array}{cccccc}
 & & & Criteria & & \\
 & C_1 & C_2 & C_3 & \dots & C_n \\
Alternatives & w_1 & w_2 & w_3 & \dots & w_n \\
A_1 & a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\
A_2 & a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\
\vdots & \vdots & \vdots & \vdots & \dots & \vdots \\
. & . & . & . & \dots & . \\
A_m & a_{m1} & a_{m2} & a_{m3} & \dots & a_{mn}
\end{array}$$

Figure 3-6 An m-by-n decision matrix

3.3.3 Weighted Product Method (WPM)

In WPM, each alternative is compared with others by multiplying a number of ratios, one for each criterion. Each ratio is raised to the power equivalent to the relative weight of the corresponding criterion. In general, in order to compare two alternatives A_K and A_L, the following product is calculated:

$$R\left(\frac{A_K}{A_L}\right) = \prod_{j=1}^{n} \left(\frac{a_{Ki}}{a_{Lj}}\right)^{w_j} \qquad \textbf{Equation 3-2}$$

where n is the number of criteria, a_{ij} is the actual value of the i^{th} alternative in term of the j^{th} criterion, and w_j is the weight of importance of the j^{th} criterion.

If the term $R\left(\frac{A_K}{A_L}\right)$ is greater than or equal to one, then it indicates that alternative A_K is more desirable than alternative A_L (in the maximization case). In IWMS modeling which is the minimization case, the opposite, i.e. alternative A_L would be more desirable than alternative A_K. For more than two alternatives MCDA minimization problem, the alternative that gives the minimum value of $R\left(\frac{A_K}{A_L}\right)$ is the best alternative.

3.4 Acquisition of parameters

Since different alternatives have different attributes or dimensions on which the decision making is based, these different attributes must be determined for each eligible alternative. As mentioned earlier, these parameters include worker exposure dose, intruder dose, CEDE at site boundary at 10000 years after disposal, costs associated with the pre-selected alternative(s) and, compatibility of the derived stream and the proposed waste form material and are considered as part of the decision making process. Some of these parameters are calculated in IWMS source code, and some of these parameters are obtained using the ORIGEN-ARP. Since the derived streams change during the course of the calculation as do their properties, IWMS automatically creates an ORIGEN input file that represent each product stream properties, calls ORIGEN (from IWMS), imports corresponding ORIGEN output back to IWMS, and utilize further those parameters for IWMS calculation. The parameters include worker exposure dose and material attractiveness. Although the material attractiveness was not used as a decision criterion, it was calculated and reported in the final outputs.

3.4.1 Worker Exposure Dose

ORIGEN output can be manipulated to a customized report of energy dependent gamma radiation intensity spectrum. However it does not report by radionuclides, instead it reports gamma emission rate (#photon/s) as a function of energy (MeV). For simplicity, the stream was assumed to be a point source in order to calculate one representative number. Gamma exposure at 1 meter (m) from the source (assumed point source) is determined and used in the decision making process. Exposure dose ($\dot{X}$) can be calculated by[57];

$$\dot{X}\left(\frac{R\,.cm^2}{hr}\right) = 1.835 * 10^{-8} \int_0^E E \left(\frac{\mu_{en}(E)}{\rho}\right)_{air} \emptyset(E)\,dE \qquad \textbf{Equation 3-3}$$

where E is energy (MeV); $\emptyset(E)$ is photon emission rate$\left(\frac{\#\gamma}{MeV-sec}\right)$; $(\rho)_{air}$ is air density ($\frac{g}{cm^3}$) and $\left(\mu_{en}(E)\right)_{air}$ is absorption coefficient in air ($\frac{cm^2}{g}$). By specifying a distance of 1 m and applying a conversion factor, the integral expression can be approximately discretized into a summation form as follows;

$$\dot{X}\left(at\ 1\ m\ in\ \frac{R}{nr}\right) = 5.2568 * 10^{-10} \sum_i^E \overline{E} * \overline{\emptyset} * \Delta E * \left(\frac{\overline{\mu}_{en}(E)}{\rho}\right)_{air} \qquad \textbf{Equation 3-4}$$

where $\overline{E}$, $\overline{\emptyset}$ and ΔE can be obtained from the ORIGEN output. The mass absorption coefficient term $\left(\frac{\overline{\mu}_{en}(E)}{\rho}\right)_{air}$ was obtained from National Institute of Standards and Technology (NIST) [58].

3.4.2 Material Attractiveness

In IWMS, the Figure of Merit (FOM) approach was used to evaluate the attractiveness of materials mixtures containing special nuclear materials (SNM) and alternate nuclear materials [59]. FOM is given by;

$$\mathrm{FOM} = 1 - log\left\{\frac{BSCM}{800} + \frac{BSCM*h}{4500} + \frac{BSCM}{50}\left(\frac{D}{500}\right)^{\frac{1}{\log 2_{10}}} + \frac{BSCM*S}{6.8*10^6}\right\} \qquad \textbf{Equation 3-5}$$

where BSCM is the bare sphere critical mass of the metal (kg), h is the heat content in ($\frac{W}{kg}$), D is the dose rate evaluated at 1 m from the surface ($\frac{rad}{hr}$) and S is the spontaneous-fission neutron production rate ($\frac{\#neutron}{sec-kg}$).

Spontaneous-fission neutron production rate is also one of the customary ORIGEN outputs, as well as heat content. The dose rate can be directly calculated from the worker dose exposure previously described. The heat content can be also obtained from ORIGEN. The bare critical mass ($BSCM$) can be calculated by a simple fitted polynomial equation as follows;

$$BSCM = 39.548 - 12.485F_{Pu239} + 101.582{F_U}^2 - 17.63F_{Pu} + 267.025F_U + 610.778{F_{Ln}}^2 - 297.808F_{Pu239}{F_U}^2 - 305.724F_{Pu}F_U - 1227.046F_{Pu}{F_{Ln}}^2$$ **Equation 3-6**

where F_{Pu} is the Plutonium (Pu) fraction to other elements, F_U is the U fraction to other elements, F_{Ln} is the Lanthanide fraction to other elements and F_{Pu239} is the Pu-239 fraction to total Pu. The equation 3-6 accounts for the stream that contains Pu, U and lanthanides, hence the stream that does not contain these materials has zero bare sphere critical mass, which results in an undefined FOM. In general the streams that contain no Pu, U or lathanides has no potential threat for a nuclear proliferation, hence a negative FOM value was assigned to this stream in order to indicate the no potential threat stream.

3.4.3 Waste Classification

The Nuclear Waste Policy Act (NWPA) defines all radioactive waste generated from UF reprocessing activities as HLW. As a consequence, it must be treated as HLW, regardless of its inherent characteristics, such as radioactivity concentration and the half-life of the materials that exist in the stream. Instead of just classifying the reprocessing product stream by its origin, one of the main objectives of the IWM concept suggested a way to reclassify the stream based on its properties. This approach should enhance an overall nuclear waste management scheme. By combining several current nuclear waste regulations with certain assumptions, the IWMS waste classification scheme was proposed and used as a basis for all relevant analyses performed by IWMS. These relevant regulations include (1) 10 CFR part 61.55 Waste Classification [60] and (2) Section 3116 in the Ronald W Reagan National Defense Authorization Act (NDAA) 2005[61]. 10 CFR part 61.55 is the classification of waste for near surface disposal. The latter regulation states the exception to the NWPA, in that all radioactive waste generated from UF reprocessing activities is HLW, except for the following government facilities: Hanford site, Savannah River site, West Valley site and

Idaho National Laboratory, if the following requirements are met. Reprocessing waste is non-HLW if such waste:

a. Does not require permanent isolation in a deep geologic repository for UF or HLW;
b. Has had highly radioactive radionuclides removed to the maximum extent; and
c. Meets the following requirements
    i. Does not exceed concentration limits for Class C LLW and will be disposed of in compliance with the performance objectives in 10 CFR Part 61 (Licensing requirements for land disposal of radioactive waste), Subpart C ; or
    ii. Exceeds concentration limits for Class C LLW but will be disposed of in compliance with the performance objectives of 10 CFR part 61, Subpart C, and pursuant to plans developed by U.S. Department Of Energy (DOE) in consultation with the U.S. Nuclear Regulatory Commission (NRC)

The performance objectives of 10 CFR Part 61, require that:

- Annual dose to a member of the public be below 25 mrem
- Intruder dose be below 500 mrem

All these requirements were translated into a simplified diagram shown in Figure 3-7.

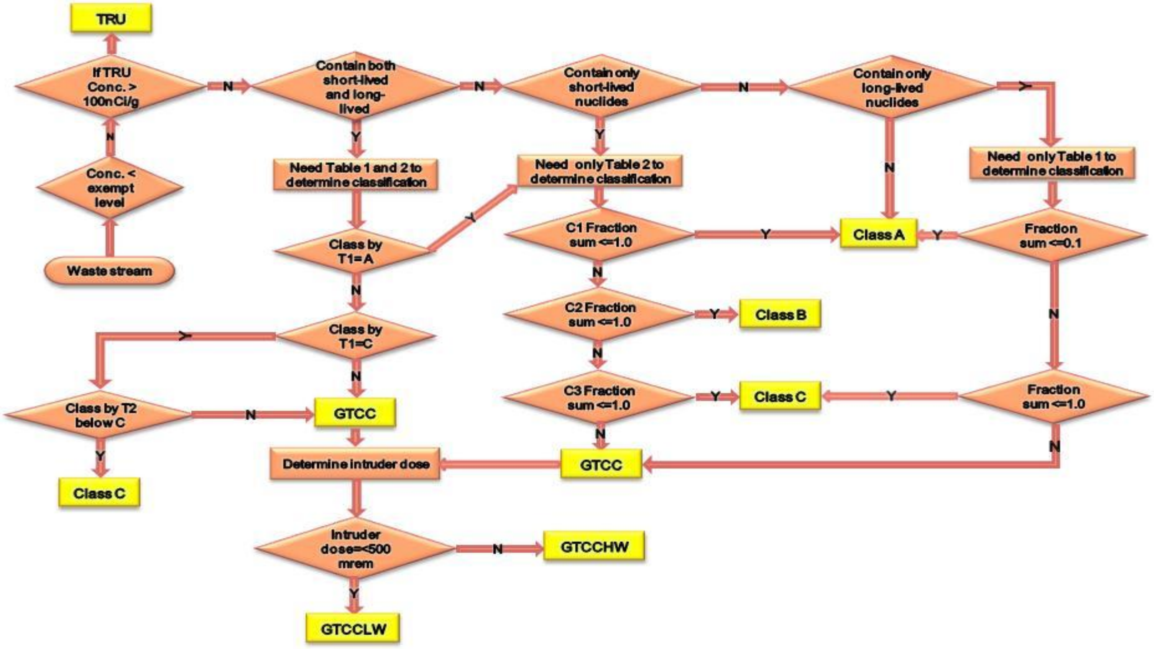


Figure 3-7 IWMS waste classification scheme

Based on Figure 3-7, each product stream is evaluated to: 1) determine if the radionuclides concentrations in the stream have exceeded the clearance level; 2) determine if the product stream contains TRU materials whose activity concentrations exceed 100 $\frac{nCi}{g}$; 3) determine if it contains radionuclides whose activity concentrations satisfy concentration limits set in either Table 1 (Figure 3-8) or Table 2 (Figure 3-9) of 10 CFR 61.55. For a stream that contains radionuclides not listed in neither Table 1 nor Table 2, it will be classified as class A LLW. For a stream that contains only radionuclides listed in Table 1, classification shall be determined as follows:

(i) If the concentration does not exceed 0.1 times the value in Table 1, the waste is Class A LLW.

(ii) If the concentration exceeds 0.1 times the value in Table 1 but does not exceed the value in Table 1, the waste is Class C LLW.

(iii) If the concentration exceeds the value in Table 1, the waste is not generally acceptable for near-surface disposal or greater than class C (GTCC) LLW.

(iv) For wastes containing mixtures of radionuclides listed in Table 1, the total concentration shall be determined by the sum of fractions rule described later in this section.

For a stream that contains only radionuclides listed in table 2, classification shall be determined as follow:

(i) If the concentration does not exceed the value in Column 1, the waste is Class A LLW.

(ii) If the concentration exceeds the value in Column 1, but does not exceed the value in Column 2, the waste is Class B LLW.

(iii) If the concentration exceeds the value in Column 2, but does not exceed the value in Column 3, the waste is Class C LLW.

(iv) If the concentration exceeds the value in Column 3, the waste is not generally acceptable for near-surface disposal or GTCC LLW.

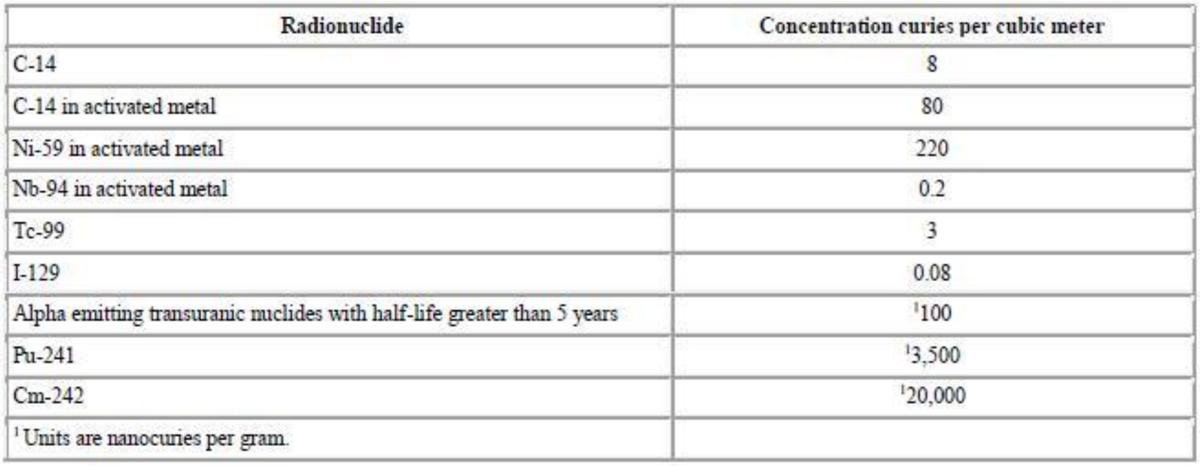
(v) For wastes containing mixtures of the nuclides listed in Table 2, the total concentration shall be determined by the sum of fractions rule

For a stream that contains radionuclides listed in both Table 1 and Table 2, classification shall be determined as follows:

(i) If the concentration of a nuclide listed in Table 1 does not exceed 0.1 times the value listed in Table 1, the class shall be that determined by the concentration of nuclides listed in Table 2.

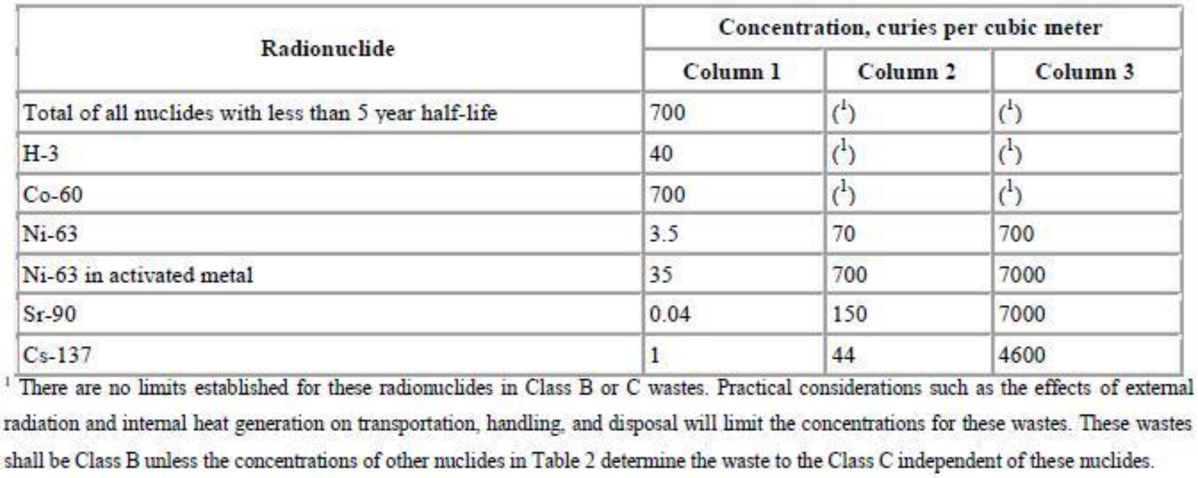
(ii) If the concentration of a nuclide listed in Table 1 exceeds 0.1 times the value listed in Table 1 but does not exceed the value in Table 1, the waste shall be Class C, provided the concentration of nuclides listed in Table 2 does not exceed the value shown in Column 3 of Table 2.

For determining the classification for waste that contains a mixture of radionuclides, it is necessary to determine the sum of fractions by dividing each nuclide's concentration by their activity concentration limits and adding the resulting values. The concentration limits must all be taken from the same column of the same table. The sum of the fractions for the column must be less than 1.0 if the waste class is to be determined by that column. Waste classification determined by 10 CFR 61.55 includes class A, B, C and GTCC. Class A, B and C waste may be disposed of at a LLW disposal facility. GTCC waste may be disposed of at a geologic repository.



Radionuclide	Concentration curies per cubic meter
C-14	8
C-14 in activated metal	80
Ni-59 in activated metal	220
Nb-94 in activated metal	0.2
Tc-99	3
I-129	0.08
Alpha emitting transuranic nuclides with half-life greater than 5 years	[1]100
Pu-241	[1]3,500
Cm-242	[1]20,000
[1] Units are nanocuries per gram.	

Figure 3-8 Table 1 of 10 CFR 61.55



Radionuclide	Concentration, curies per cubic meter		
	Column 1	Column 2	Column 3
Total of all nuclides with less than 5 year half-life	700	(1)	(1)
H-3	40	(1)	(1)
Co-60	700	(1)	(1)
Ni-63	3.5	70	700
Ni-63 in activated metal	35	700	7000
Sr-90	0.04	150	7000
Cs-137	1	44	4600

[1] There are no limits established for these radionuclides in Class B or C wastes. Practical considerations such as the effects of external radiation and internal heat generation on transportation, handling, and disposal will limit the concentrations for these wastes. These wastes shall be Class B unless the concentrations of other nuclides in Table 2 determine the waste to the Class C independent of these nuclides.

Figure 3-9 Table 2 of 10 CFR 61.55

In the next step, all waste streams that are classified as GTCC LLW, will be further evaluated using the intruder dose approach. Should the stream exhibit less than or equal to 500 mrem intruder dose for intruder drilling scenarios, that particular stream may be disposed of as class C LLW. Here, the new acronym "GTCCLW" is used throughout this document to refer to this waste classification. Should the stream exhibit more than 500 mrem intruder dose for intruder drilling scenarios, it may be disposed of at a deep geological repository. The acronym for this waste classification is "GTCCHW". Because US practices utilize LLW disposal facility acceptance requirements, i.e. both origin and property of the waste packages vary in different states, hence an essential assumption required here is that the prospect waste packages produced from reprocessing process can be disposed of at the Andrews site, Texas for all LLW and MLLW and YM disposal facilities for all GTCCHW and TRU.

3.4.4 Volume of Conditioned Waste Forms

Although all available non-exempt alternatives have direct disposal as a final destination, a comprehensive waste volume calculation scheme was applied for only direct disposal and partial disposal under the decontamination and recycle option. A couple of reasons exist for this. For radionuclide transmutation, data on transmutation products are either unavailable or do not exist, because the transmutation products usually depend on various factors such as type, energy and flux of the particle bombarding the nuclide of interest or transmutation targets that are not yet well established. The amount of unprocessed waste volume resulting from the transmutation option was assumed for completeness of modeling. More detailed information could be updated once it is available. For the decay storage option, future treatment technology is required for an actual analysis. Since there is no information on this topic, current technology was applied to calculate the conditioned waste volume for this option.

Common products from waste treatment and conditioning facility are conditioned waste forms or simply waste forms. Conventional final waste forms are vitrified glass, ceramics or metal for HLW and concrete, metal or polymer for LLW. With appropriate pretreatment/treatment that is typically designed for volume reduction of an incoming waste stream (usually dependent on physical and chemical forms of the as-generated waste) and maximum waste loading in certain waste forms, final waste forms volume can be determined. A simple waste treatment and conditioning scheme used in IWMS modeling is shown in Figure 3-10. Each of the as-generated waste streams is pretreated/treated based on its properties, i.e. whether it is Dry Active Waste (DAW), liquid waste, wet solid waste or metal waste. In IWMS calculation, this treated waste volume is not affected by waste classification, only by the physical properties reflected by its type. A representative volume reduction ratio for each waste category was used in the modeling to calculate the treated volume of the incoming waste stream. Depending on the waste form material to be used as immobilizing material, waste loading of the treated waste in certain waste form was used to calculate the final waste form volume. Except for the amount of waste loading in glass waste form that is calculated based on the amount of certain elements, such as Sulphur, Chromium, Rhuthenium, Molybdenum, Palladium, that exist in the waste stream, the waste loading percentage in other waste forms was fixed and hence is required as an input parameter. Both volume reduction ratio and percent waste loading are required for the calculation. Their input interfaces are located in the MS Excel spreadsheet named “Wasteforms”. In the modeling, different waste classifications and waste packaging were accounted for through the manufacturing cost of waste forms (which are also required as an input parameter).

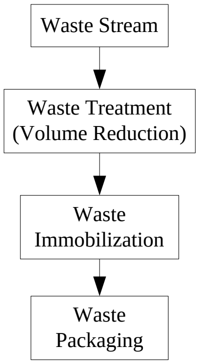


Figure 3-10 IWMS waste handling diagram

By regulation, the final waste form that is permanently disposed in its designated repository must be evaluated to ensure the safety to both humans and the environment in short and long term. A quantitative evaluation, called performance assessment, is performed to evaluate the radiological dose for this purpose [62]. Due to many restrictions set in this evaluation, only some important parameters, i.e. intruder dose and CEDE at 10000 years after the closure of the disposal site, were used in this research.

3.4.5 Intruder Dose

As part of the performance objectives set forth in 10 CFR Part 61, protection of individuals from inadvertent intrusion needs to be addressed and satisfied. Design, operation, and closure of the land disposal facility must ensure protection of any individual inadvertently intruding into the disposal site and occupying the site or contacting the waste at any time after active institutional controls over the disposal site are removed [63]. Dose to an intruder (intruder dose) into a waste-disposal site was used as one of IWMS waste management decision criteria. FORTRAN code developed by Steve Fetter [64] was used for this modeling part. The methodology in the code closely resembled that used in the Draft Environmental Impact Statement on 10 CFR Part 61[65], although it is not identical. The differences between 10

CFR Part 61 and this code are pathway dose conversion factors (PDCF) and shielding factors. These differences were not significant considering the final results are to be used in relative comparison between alternatives in the same waste stream. This code was converted from FORTRAN77 into FORTRAN 90 and integrated into the IWMS source code.

3.4.6 Committed Effective Dose Equivalent (CEDE)

As part of the performance assessment, a combination of radiological dose at the nearest possible access location from all possible environmental pathways must be calculated. For simplification, only the ingestion pathway (drinking water from the well that is connected to the contaminated underground water) was considered in IWMS modeling because it is considered the most relevant to radioactive waste disposal. CEDE ($\frac{mrem}{y}$) at the nearest possible access location only at 10000 years after site closure was used as a decision criteria in both decision making level. It can be expressed by:

$$\boldsymbol{CEDE = \sum_{i=1}^{N} Conc_i * \left(DCF_{ing}\right)_i * I} \qquad \textbf{Equation 3-7}$$

where $Conc_i$ is the concentration of radionuclide i ($\frac{Ci}{m^3}$) at the nearest possible access location at 10000 years after site closure, $\left(DCF_{ing}\right)_i$ is the committed effective ingestion dose conversion factor [66] of radionuclide i ($\frac{mrem}{Ci}$) and I is ingestion rate. In this model, water consumption rate of 0.5 $\frac{m^3}{y}$ was used [67]. The assumption made here is that human behaviors (i.e. drinking habits and health responses to radiation) 10000 years in the future would remain the same as the current day.

Note that during separation, radiological decay was not taken in account because the entire reprocessing scheme for UF is generally in an order of weeks or at most months. UF is usually kept for a certain period of time for cooling right after its discharge from nuclear reactor, which allows short-lived radionuclides to decay away. It is reasonable to assume that there is no decay during separation, but for the 10000 years' time frame, radiological decay of the existing radionuclides in the waste stream must be taken into account.

To determine radionuclides concentrations in groundwater at specific time and location, one needs to solve partial differential equations (time and space variable). Solving these equations usually takes time. In IWMS, space and time were assumed to be independent of each other so that simpler methodologies could be applied in order to save the calculation time. The time evolution of nuclide concentrations undergoing serial or linear decay chain is governed by a set of first-order ordinary differential equation, called the Bateman equations. The analytical solution of the Bateman equations for the case of radioactive decay in a linear chain is given by H. Bateman [68]. For a complex system such as radioactive waste disposal which is composed of approximately hundred radionuclides that could transform into other radionuclides that already exist in the system, simplification has to be made. This simplification includes (1) ignoring relatively short-lived radionuclides in decay chains and (2) considering only the decay chains that contain radionuclides that contribute to CEDE calculation. In IWMS, 7 decay chains (Figure 3-11) were assumed based on the list of relevant radionuclides given in the Appendix F.

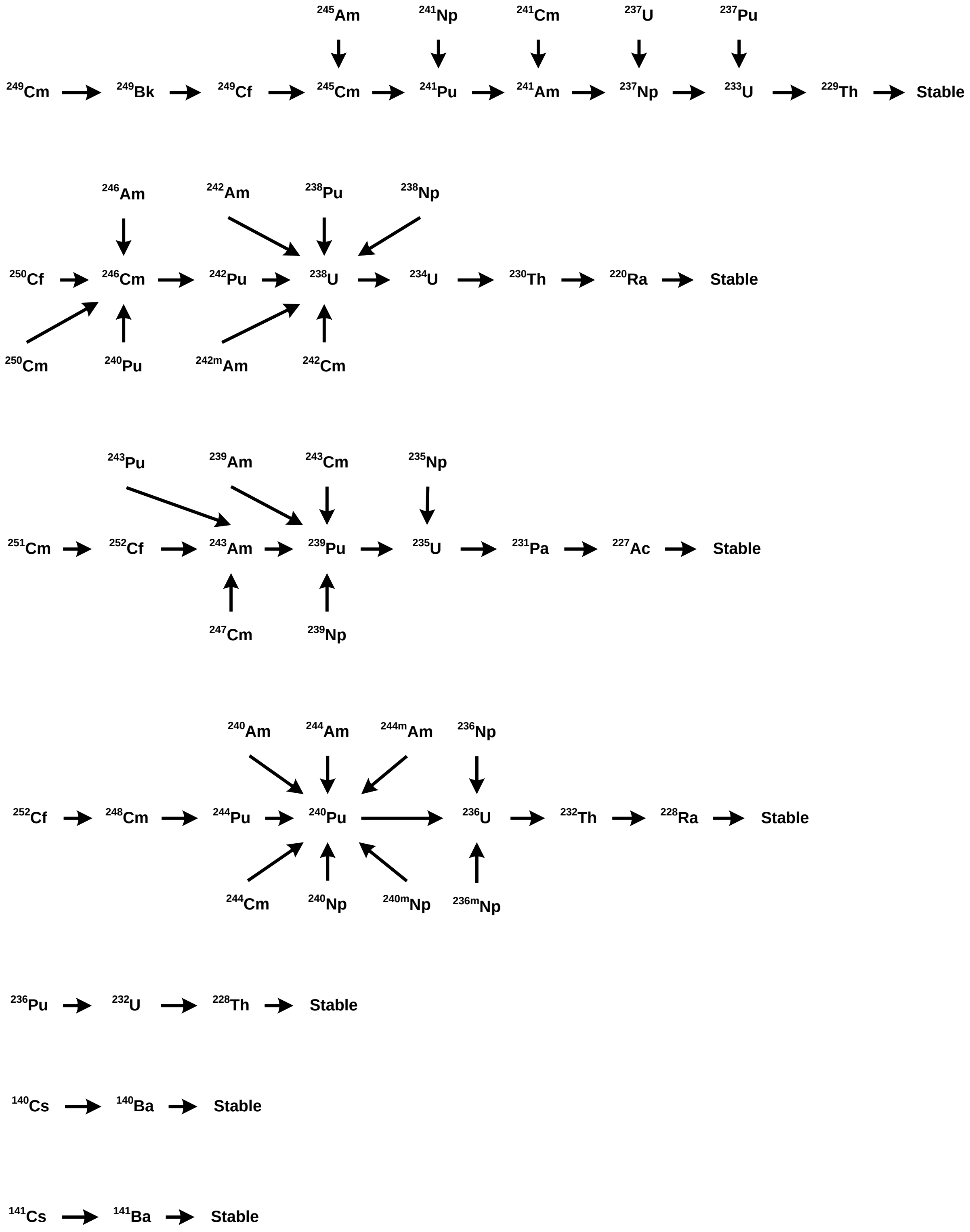


Figure 3-11 Decay chain number 1 to 7 considered in IWMS modeling

The Bateman equation can be used to count for the inventory of nuclide at time t (y). It can be written as:

$$\boldsymbol{N_{ij} = N_{i0} \prod_{k=i}^{j-1} \lambda_k \sum_{L=1}^{j} \frac{e^{-\lambda_L t}}{\prod_{\substack{m=i \\ m \neq L}}^{j} (\lambda_m - \lambda_L)}} \qquad \textbf{Equation 3-8}$$

where N_{ij} is the contribution from the i^{th} chain member to the j^{th} chain member, N_{i0} is the initial mass of the ith chain member, and λ_j is the decay coefficient of the j^{th} chain member. The total amount of the j^{th} chain member at time t is:

$$\boldsymbol{N_j = \sum_{i=1}^{j} N_{ij}} \qquad \textbf{Equation 3-9}$$

Another important factor in determining the dose resulting from waste disposal is source term evaluations. Source term or rate of radionuclide released ($Q_0(t)$) means the actual radionuclides concentrations that release from the waste forms and container simultaneously. The source term is usually expressed as a function of time. Assumptions of the determination of the source term vary greatly depending on the waste classification of the buried wastes. The general assumption for all LLW disposals is that the LLW container fails right after disposal and allows all the radionuclides distributed inside the container to release to the environment. Since a typical LLW facility is located in an unsaturated zone, first the released radionulclides dominantly transport in the vertical direction (they also move horizontally but significantly less compared to vertical transport) until they reach the water table and merge with the aquifer in the saturated zone which subsequently starts to move dominantly in the horizontal direction. Figure 3-12 illustrates this process.

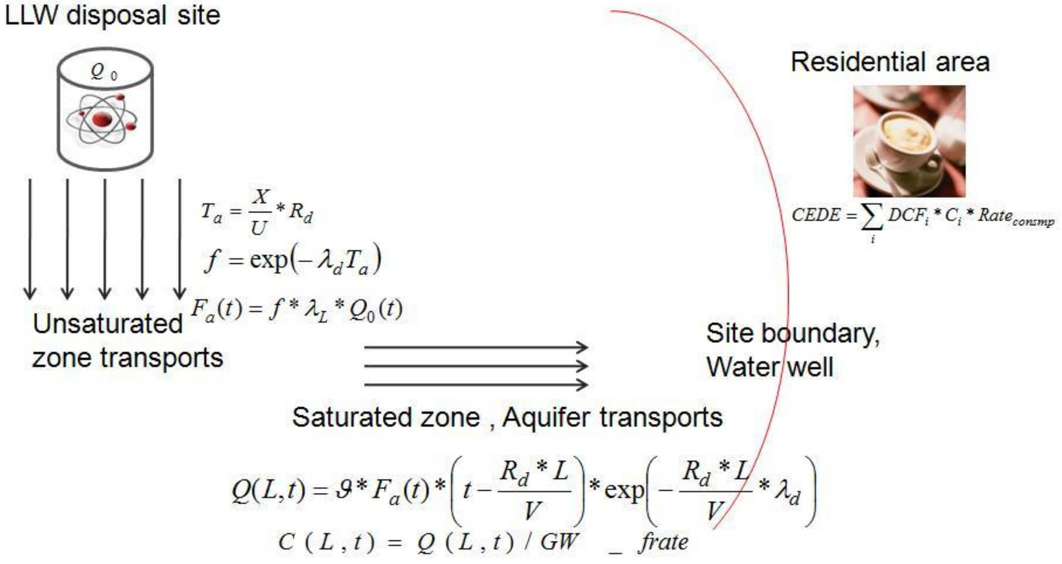


Figure 3-12 Radionuclides transport from LLW disposal

In order to determine radionuclides concentrations at the location of interest, groundwater transport models for both unsaturated and saturated zones are needed. For unsaturated zone transport, the GWSCREEN unsaturated zone transport model [69] was adopted. The plug flow model was used for the vertical unsaturated zone in the GWSCREEN code. In the plug flow model, the amount of decay that occurs during the transit time is a function of the contaminant transit time in the unsaturated zone. The transit time in the unsaturated zone (T_a) is given by the following:

$$\boldsymbol{T_a = \frac{X}{U} * R_d} \qquad \textbf{Equation 3-10}$$

where X is the distance from the base of the source volume to the top of the aquifer (m), U is the unsaturated pore velocity ($\frac{m}{y}$), and R_d is the retardation factor in the unsaturated zone. The pore velocity is given by:

$$\boldsymbol{U = \frac{P}{\theta}} \qquad \textbf{Equation 3-11}$$

where θ is the volumetric water content in the unsaturated zone ($\frac{m^3}{m^3}$), and P is percolation at the site ($\frac{m^3}{y}$). The retardation factor is given by:

$$R_d = \frac{n}{n_e} + \rho * \frac{k_d}{n_e} \qquad \textbf{Equation 3-12}$$

where k_d is distribution coefficient ($\frac{mg}{L}$), ρ is bulk density ($\frac{mg}{L}$), n is porosity and n_e is effective porosity. The fraction of mass or activity that remains after transit through the unsaturated zone (f) is given by:

$$f = e^{-\lambda_d T_a} \qquad \textbf{Equation 3-13}$$

The contaminant flux to the aquifer (F_a) is given by:

$$F_a = f * \lambda_L * Q_0(t) \qquad \textbf{Equation 3-14}$$

where λ_L is the leaching rate constant (per year).

For the saturated zone transport model, the correlation developed by Hung[70] was used. The governing equation is shown as follows:

$$Q(t) = \vartheta * Q_0\left(t - \frac{R_d * L}{V}\right) * \exp\left(-\frac{R_d * L}{V} * \lambda_d\right) \qquad \textbf{Equation 3-15}$$

$$\vartheta = \frac{\exp\left(\frac{P_t}{2}\left(1 - \sqrt{1 + \frac{4R_d L}{v} * \frac{\lambda_d}{P}}\right)\right)}{\exp\left(-\frac{R_d * L}{V} * \lambda_d\right)} \qquad \textbf{Equation 3-16}$$

where $Q(t)$ ($\frac{Ci}{y}$) denotes the rate of radionuclide transport at the receptor location, R_d is the retardation factor (see Equation 3-12), L is a physical distance between source and receptor location (m), λ_d is radiological decay constant, V is the interstitial velocity ($\frac{m}{y}$), ν is the velocity of nuclide in the fluid ($\frac{m}{y}$), and P_t is the Peclet number.

$$P_t = \frac{VL}{D} \qquad \textbf{Equation 3-17}$$

where L is the receptor distance (m), D is the diffusion coefficient ($\frac{m^2}{y}$)

$$V = \frac{\nu}{n} \qquad \textbf{Equation 3-18}$$

$$\nu = -K \frac{\frac{\partial H}{\partial X}}{n} \qquad \textbf{Equation 3-19}$$

where $\frac{\partial H}{\partial X}$ is the water table slope ($\frac{m}{m}$), and K is the hydraulic conductivity ($\frac{m}{y}$). Radionuclide concentration ($\frac{Ci}{m^3}$) is the required parameter to calculate CEDE. To convert from the rate of radionuclide transport to radionuclide concentration, simply divide the rate of radionuclide transport by underground water discharge or volumetric flow rate ($\frac{m^3}{y}$) .

$$\boldsymbol{C(t) = \frac{Q(t)}{GW_{F\_rate}}}$$ **Equation 3-20**

Unlike the LLW container, a HLW container usually has more integrity than the LLW one. For HLW disposal, it is reasonable to assume a time lag from an initial disposal to the failure of waste container. Time to container failure of 1000 years was assumed [71]. A borosilicate glass waste form, a typical waste form of HLW, or a ceramics waste form is not normally dissolved in groundwater easily. If the waste form is still intact, the radionuclides existed in the waste form will not release. As a result, they could not transport to location of interests and consequently contribute to the CEDE. It is reasonable to assume this mechanism in the overall groundwater transport process. Hence, in IWMS, dissolution from glass, ceramics and metal waste forms for HLW disposal were considered. They are briefly described in later section in this chapter.

A typical assumption regarding HLW transport is that the repository location is located right at the aquifer (HLW repository was assumed to be located in a saturated zone,) i.e. not considering a travel time in unsaturated zone. Since the IWMS modeling assumes that the YMF is the geological repository, and this facility is located in the unsaturated zone, it is reasonable to incorporate the travel time in the unsaturated zone. Figure 3-13 shows a conceptual model for radionuclides released from the HLW. The plug flow model was used in the unsaturated zone transport calculation. For the saturated zone transport calculation, the correlation developed by Hung [70] was used.

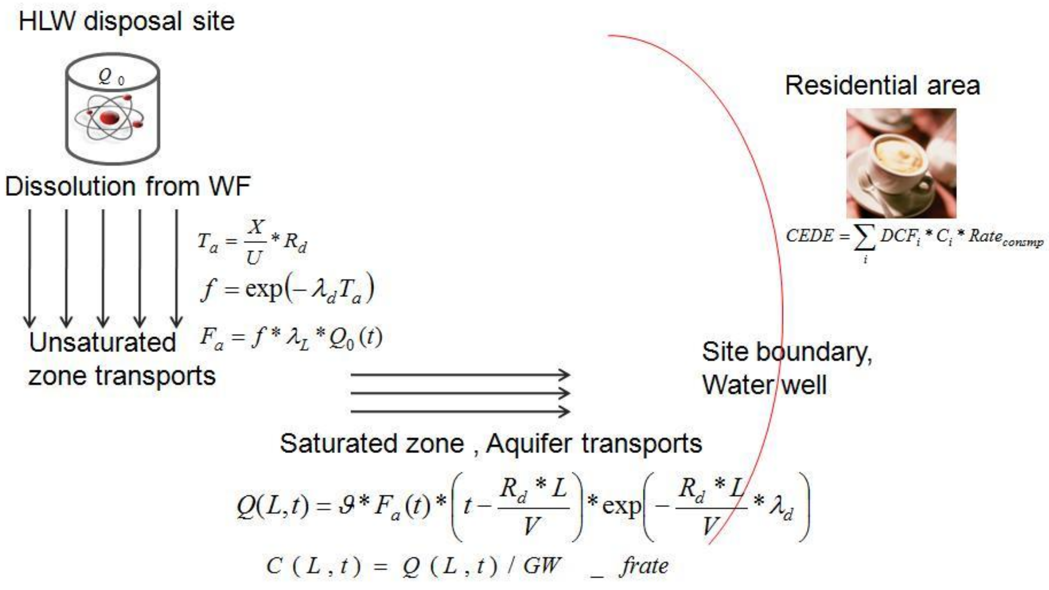


Figure 3-13 Radionuclides transport from HLW disposal

3.4.6.1 Glass source term modeling

In IWMS, a simplified glass dissolution model can be expressed by:

$$\boldsymbol{r_g = k_0 10^{\eta pH} e^{-\frac{E_a}{RT}}} \qquad \textbf{Equation 3-21}$$

where r_g is the dissolution rate ($\frac{g}{m^2-y}$), k_0 is the intrinsic dissolution rate, η is the pH dependence factor, E_a is the activation energy, pH is the pH of the solution, and T is temperature (K) of the solution. The dissolution rate of glass is multiplied with an effective specific surface area a_{glass} in units of ($\frac{m^2}{g}$) to calculate the fractional release of glass. The dissolution rate of the glass (r_m) form waste for a loading of m (kg) glass form waste is calculated by:

$$\boldsymbol{r_m = r_g * a_{glass} * m} \qquad \textbf{Equation 3-22}$$

The parameters used in the glass dissolution section were obtained from [72].

3.4.6.2 Ceramics source term modeling

The governing equation for the ceramic dissolution rate is similar to the glass waste form [72], with different parameters such as intrinsic dissolution rate, pH dependence factor, activation energy, and specific surface area. These parameters were also obtained from the reference [72].

3.4.6.3 Metal source term modeling

For the metal source term calculation, a model proposed by Bauer, T.H. et. al. [73] was used to calculate the release rate from metal. The model expresses the release rate in term of the bounding release rate (r_b) ($\frac{g}{m^2-y}$) that can be written as:

$$\boldsymbol{r_b = \frac{a_{max}\ln\left(1+\frac{b*a_{max}}{a_{max}}*365*T_s\right)}{T_s}} \qquad \textbf{Equation 3-23}$$

where r_g is the bounding release rate from metal ($\frac{g}{m^2-y}$), T_s is the size of the time duration of actual immersion experiment (1 y was conservatively assumed), a_{max} ($\frac{g}{m^2}$) and b*a_{max} ($\frac{g}{m^2-day}$) are fitted parameters that represent the conceptually significant bounding quantities of “passivation onset” and “initial release rate”. These parameters depend on pH and temperature and chloride concentration, and can be determined as follows:

$$\boldsymbol{\ln(b*a_{max}) = -0.54624 - 0.69046\,pH + (0.019665 + 5.8415E-6*[Cl])*T} \qquad \textbf{Equation 3-24}$$

$$\boldsymbol{\ln(a_{max}) = 7.9812 + 2.3938E-4*[Cl] - 1.2273*pH} \qquad \textbf{Equation 3-25}$$

3.4.6.4 Nuclide inventory in groundwater

Once the dissolution rate is determined, the radionuclide that can be released from the waste package to the water in the waste package can also be determined (assuming water can penetrate the waste package in case of failure). The governing equation is given by:

$$\boldsymbol{\frac{dm_i}{dt} = w_{li}(t) - w_{ci}(t) - m_i\,\lambda_i + m_{i-1}\lambda_{i-1}} \qquad \textbf{Equation 3-26}$$

where m_i is the mass of the *i*th nuclide (Ci), λ_i is the decay constant of the *i*th nuclide (1/y), m_{i-1} is the mass of the parent nuclide of the *i*th nuclide (Ci), λ_{i-1} is the decay constant of the parent of the *i*th nuclide (1/y), $w_{li}(t)$ is leach rate of the *i*th nuclide from waste form to water in the waste package ($\frac{Ci}{y}$) which can be determined from dissolution rate of the waste form material of interest, $w_{ci}(t)$ is leaching rate of the *i*th nuclide from water in the waste package to the near environment ($\frac{Ci}{y}$).

Only advective mass transfer out of the waste package is considered and represented by the following equation, hence

$$\boldsymbol{w_{ci}(t) = C_i(t) * q_{out}(t)} \qquad \textbf{Equation 3-27}$$

The concentration $C_i(t)$ is determined by dividing the mass of nuclide *i* with volume of water in the waste package (V_{wp}), and $q_{out}(t)$ is the rate at which water leaves the waste package at time ($\frac{m^3}{y}$). Substitute $w_{ci}(t)$ and assume that $q_{out}(t)$ and $w_{ci}(t)$ are constant during calculation time step. Then the governing equation becomes:

$$\boldsymbol{\frac{dm_i}{dt} = w_{li} - C_i(t) * q_{out} - m_i\,\lambda_i + m_{i-1}\lambda_{i-1}} \qquad \textbf{Equation 3-28}$$

The concentration of nuclide *i* depends on the solubility limit of nuclide *i* (sol_i) in waste package water. It can be determined according to the solubility limit as follows:

$$\boldsymbol{C_i(t) = \begin{cases} \frac{m_i}{V_{wp}} & if\ \frac{m_i}{V_{wp}} \le sol_i \\ sol_i & otherwise \end{cases}} \qquad \textbf{Equation 3-29}$$

Hence we have governing equations for the nuclides with and without solubility limit as follows:

$$\boldsymbol{\frac{dm_i}{dt} = w_{li} - sol_i * q_{out,j} - m_i\,\lambda_i + m_{i-1}\lambda_{i-1}} \qquad \textbf{Equation 3-30}$$

$$\boldsymbol{\frac{dm_i}{dt} = w_{li} - \frac{m_i * q_{out,j}}{V_{wp}} - m_i\,\lambda_i + m_{i-1}\lambda_{i-1}} \qquad \textbf{Equation 3-31}$$

The solution to the system has 4 different forms:

(1) The solution for the parent nuclide when its concentration is lower that its solubility limit is given by:

$$m_i(t) = m_i(t_{j-1}) * \mathrm{e}^{-\left(\frac{q_{out,j}}{V_{wp}}+\lambda_i\right)*(t-t_{j-1})} + \frac{\mathrm{w_{i,j}}}{\frac{q_{out,j}}{V_{wp}}+\lambda_i} * \left(1 - \mathrm{e}^{-\left(\frac{q_{out,j}}{V_{wp}}+\lambda_i\right)*(t-t_{j-1})}\right) \quad \textbf{Equation 3-32}$$

(2) The solution for the parent nuclide when its concentration is limited by its solubility limit is given by:

$$m_i(t) = m_i(t_{j-1}) * \mathrm{e}^{-\lambda_i*(t-t_{j-1})} + \frac{\mathrm{w_{i,j} - sol_i * q_{out,j}}}{\lambda_i} * \left(1 - \mathrm{e}^{-\lambda_i*(t-t_{j-1})}\right) \qquad \textbf{Equation 3-33}$$

(3) The solution for the daughter nuclide when its concentration is lower that its solubility limit is given by:

$$m_i(t) = m_i\left(t_{j-1}\right) + \frac{\mathrm{w_{i,j}} - \left(\frac{q_{out,j}}{V_{wp}}+\lambda_\mathrm{i}\right) * \mathrm{m_{i,j-1}} + \lambda_\mathrm{i-1}\mathrm{m_{i-1,j}}}{1 + \left(\frac{q_{out,j}}{V_{wp}}+\lambda_i\right)*(t-t_{j-1})} * \left(t - t_{j-1}\right) \qquad \textbf{Equation 3-34}$$

(4) The solution for the daughter nuclide when its concentration is limited by its solubility limit is given by:

$$m_i(t) = m_i\left(t_{j-1}\right) + \frac{\mathrm{w_{i,j} - sol_i * q_{out,j}} - \lambda_\mathrm{i}\mathrm{m_{i,j-1}} + \lambda_\mathrm{i-1}\mathrm{m_{i-1,j}}}{\lambda_i} * \left(t - t_{j-1}\right) \qquad \textbf{Equation 3-35}$$

3.5 IWMS Input and Output Parameters

3.5.1 IWMS Input Parameters

Input parameters are defined as information that must be imported to IWMS code, and can be divided into two types, based on level of the uncertainty, i.e. parameters with large uncertainty and less uncertainty. The large uncertainty data were listed in MS Excel spreadsheets where the user-interfaces are located as explained earlier in this chapter. These input parameters are exported into text files and organized into specific folders, with details given in Appendix D. The small uncertainty data were located inside the main IWMS code in FORTRAN format (please see the complete list in Appendix E), and they could not be altered during the calculation. Examples of major input parameters of UREX process are given in this section. UREX process flow parameters [17], unit secondary waste generation are given in Table 3-2 and Table 3-3 and Table 3-4, respectively. Since all of the advanced aqueous separation processes only exist in laboratory demonstration scale, cost data (capital, operation, maintenance cost and decommissioning costs) for all these processes were approximated from PUREX process (the only process that exists commercially) [74 ,75]. These cost data were estimated in 1975 US dollars and appropriate inflation rates were applied to these data. Estimated cost data are given in Table 3-5. Some of the input parameters that are not addressed in this section are located in FORTRAN part which details can be found in Appendix E and F.

Table 3-2 UREX process flow parameters required by IWMS modeling

Description	**Variable**	**(L/L Aq. feed)**
Volume ratio of minimum required TBP	Vol_TBP	1.05E+00
Volume ratio of minimum required Dodecane	Vol_Dod	2.46E+00
Volume ratio of 0.3 M HNO3 scrub	Vol_Dscr_HNO3	5.79E-01
Volume ratio of 0.01 M HNO3 U strip	Vol_Dstr_HNO3	3.51E+00
Volume ratio of 6.0 M HNO3 Tc strip	Vol_Hstr_HNO3	9.65E-01
Volume ratio of diluted HNO3 Wash solution	Vol_Dwas_HNO3	1.50E+00
Volume ratio of AHA	Vol_AHA	4.70E-01
U Fraction distributed in wash effluent	WASH_EFF_U	5.00E-07
Description	**Variable**	**(L/L Aq. feed)**
Tc Fraction distributed in wash effluent	WASH_EFF_Tc	5.00E-07
U Fraction distributed in spent solvent	SPNT_EFF_U	1.00E-06
Tc Fraction distributed in spent solvent	SPNT_EFF_Tc	1.00E-06
Fraction of activity subjected to contribute to 2nd waste	F_SW	1.00E-07
Fraction of activity subjected to contribute to solvent	F_SOLV	1.00E-06

Table 3-3 UREX process raw materials costs required by IWMS modeling

Unit cost for UREX raw materials	**Variable**	**(USD/L)**
30% TBP	Cost_TBP	3.80E+01
70% Dodecane	Cost_Dod	2.53E+04
1.0 M HNO3 Feed	Cost_HNO3	8.32E+00
0.01 M HNO3 U strip	Cost_HNO3	8.32E-02
6.0 M HNO3 Tc strip	Cost_HNO3	4.99E+01
1.0 M HNO3 Wash solution	Cost_HNO3	8.32E-02
0.47 M AHA	Cost_AHA	4.15E+02

Table 3-4 Secondary waste generated by UREX process

Waste type	Volume*(L/kgUO2)	Density(kg/L)	Activity fraction**
UREXMetal	0.0000E+00	7.8740E+00	0.0000E+00
UREXLiq_Aq	3.5787E-02	1.0000E+00	8.0000E-01
UREXLiq_Or	1.5284E-02	7.5000E-01	1.0000E-01
UREXSludge	0.0000E+00	2.0000E+00	0.0000E+00
UREXResin	0.0000E+00	7.0000E-01	0.0000E+00
UREXFilter	5.4233E-01	1.6400E+00	2.0000E-02
UREXTech	5.4233E-01	3.0000E+00	4.0000E-02
UREXEquip	5.4233E-01	1.2300E+00	4.0000E-02
UREXAsh	0.0000E+00	1.5000E+00	0.0000E+00
UREXMixed	0.0000E+00	1.0000E+00	0.0000E+00
UREXMisc1	0.0000E+00	1.0000E+00	0.0000E+00
UREXMisc2	0.0000E+00	1.0000E+00	0.0000E+00

Table 3-5 Unit costs for head-end, separation and support processes (2010 USD)

Process	O&M Cost	Capital Cost	Decommissioning Cost	Total Cost
DISB	2.07E+03	3.45E+04	9.80E+02	3.76E+04
CHOP	2.07E+03	3.45E+04	9.80E+02	3.76E+04
VOLX	2.07E+03	3.45E+04	9.80E+02	3.76E+04
DISSV	2.07E+03	3.45E+04	9.80E+02	3.76E+04
DISSC	2.07E+03	3.45E+04	9.80E+02	3.76E+04
UREX	2.07E+03	3.45E+04	9.80E+02	3.76E+04
COEX	2.07E+03	3.45E+04	9.80E+02	3.76E+04
FPEX	2.07E+03	3.45E+04	9.80E+02	3.76E+04
CCDPEG	2.07E+03	3.45E+04	9.80E+02	3.76E+04
TRUEX	2.07E+03	3.45E+04	9.80E+02	3.76E+04
TALSPEAK	2.07E+03	3.45E+04	9.80E+02	3.76E+04
REVTAL	2.07E+03	3.45E+04	9.80E+02	3.76E+04
MOXFUEL	1.00E+03	1.67E+03	9.29E+03	1.20E+04
NEXFUEL	1.10E+03	1.83E+03	1.02E+04	1.32E+04
OFGTV	2.07E+03	3.45E+04	9.80E+02	3.76E+04
OFGTC	2.07E+03	3.45E+04	9.80E+02	3.76E+04

The UF inventories and target separation efficiencies are also located in MS Excel spreadsheet AFC-IWMS for easy manipulation. Radioactivity concentration (*Ci*), mass (*kg*), air toxicity (m^3 *air*), water toxicity (m^3 *water*) and heat output (*Watts*) of radionuclides of interest in UF were calculated by ORIGEN-ARP as part of SCALE 6 software [76]. These values, along with their radiological half-lives (year) and committed effective dose conversion factors (Sv/Bq) [66], were fed as part of the input parameters. Complete lists of radionuclides considered in IWMS are given in appendix F.

In the main interface, input parameters were distributed between eleven different spreadsheets: namely “AFC-IWMS”, “Reprocessing System”, “Cost”, “Top_level”, “Sub_level”, “2nd_waste”, “Wasteforms”, “HeadendParameters”, “SeparationParameters”, “SupportParameters” and “GroundWaterTransport”. There are also two more spreadsheets named “StreamAlternative” and “Freespace” which serve as a workspace for importing calculation results. The spreadsheet named “IWMS-AFC” serves as the main output summary report. Descriptions for each sheet are briefly explained below:

3.5.1.1 Input parameters in spreadsheet “AFC-IWMS”

Details in this spreadsheet include radionuclides inventories in given UF and target recovery efficiency. Appendix F1, F2 and F3 list all radionuclides considered in this research. In this research, 3 percent enrichment PWR 17x17 Westinghouse fuel assemblies from Turkey Point 3 nuclear power plant were used as a test case fuel. This UF assembly was irradiated in the reactor for 3 different cycles. The total fuel burnup was 45 MegaWatt Day per Metric ton Uranium (MWD/MTU). This specific assembly was discharged from the reactor in November 1975. More detailed information on this UF assembly such as fuel compositions, cladding compositions and reactor core up and down times were given in NUREG/CR5625 [77]. These data were used to create ORIGEN-ARP input file. Next, radionuclides inventories were determined and used as part of the IWMS input parameters. These inventories are shown in Appendix F.

3.5.1.2 Input parameters in spreadsheet “Reprocessing System”

This sheet consists of the locations where user can: (1) enter a desired reprocessing scheme such as UREX, UREX+1, UREX+1a and etc; (2) specify which type parameter will be subjected to probabilistic analysis using @Risk software; (3) manually export MS Excel based input parameters into the format required by the main calculation code and (4) simulate a single calculation or multiple calculation if using @Risk software. A benchmarking case reprocessing scheme was a series that contains disassembling, chopping, dissolution and adjusted COEX (to mimic PUREX process) processes.

3.5.1.3 Input parameters in spreadsheet "Cost"

Unit costs (capital, operation and maintenance, decommissioning and total costs) for the process employed under advanced reprocessing, i.e. head-end, separation and support processes, in USD are provided in the spreadsheet. The estimated cost data for capital, operation and maintenance, and decommissioning of the UREX+1a was obtained from the reference [4]. A Typical UREX process in the literature includes also head-end (disassembling, chopping and dissolution) and off-gas treatment (IWMS defined support process). The total cost provided in the document was equally divided into head-end (disassembling, chopping and dissolution or DISB, CHOP and DISSC respectively), separation (UREX, CCD/PEG, TRUEX and TALSPEAK) and support processes (off-gas treatment or OFGTC) shares. For all other separation processes (COEX, FPEX and reverse TALSPEAK), the cost data were assumed to be the same as the separation share previously calculated. The cost of the next generation fuel fabrication process was estimated from the cost of the MOX fuel fabrication process [4]. Since all the cost data in the reports were estimated as of 2009, an appropriate inflation rate[ee] was applied to obtain the current dollar values. Table 3-6 provides the calculated costs based on the previous estimations.

Table 3-6 Unit cost for reprocessing process of UF (USD/ MTU)

Process box	O&M Cost	Capital Cost	Decommissioning Cost	Other Cost	Total Cost
DISB	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
CHOP	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
VOLX	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
DISSV	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
DISSC	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
UREX	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06

[ee] http://inflationdata.com/inflation/Inflation_Calculators/Inflation_Calculator.asp#calcresults

Table 3-6 Continued

Process box	O&M Cost	Capital Cost	Decommissioning Cost	Other Cost	Total Cost
COEX	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
FPEX	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
CCDPEG	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
TRUEX	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
TALSPEAK	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
REVTAL	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
MOXFUEL	8.13E+02	8.13E+02	8.13E+02	8.13E+02	3.25E+03
NEXFUEL	8.94E+02	8.94E+02	8.94E+02	8.94E+02	3.58E+03
OFGTV	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06
OFGTC	1.96E+06	3.94E+04	2.65E+05	2.26E+06	4.52E+06

3.5.1.4 Input parameters in spreadsheet “2nd_waste”

This sheet describes the amount of secondary waste associated with the processes, i.e. head-end, separation and support processes, employed in IWMS modeling. A report on waste treatment at the La Hague and Marcoule Sites in France [78] was used as a basis for secondary waste estimation for IWMS modeling. Both sites have been operating UF reprocessing using the PUREX process. There are waste treatment facilities located nearby to treat waste streams from the reprocessing plants. In this research, UF was assumed to be intact (i.e. no rupture) and the metal scrap from chopping process was used in the dissolution process as well as fuel hulls (chopped fuels). Based on the assumptions, there would be no secondary waste from disassembling and chopping processes. According to the report, unprocessed waste streams from the PUREX process were generally lumped together before sending the stream to waste treatment plants, hence estimation using the sharing (between sub-processes) approach was used. From the report, the unprocessed wastes were not addressed directly, at least volume-wise; instead volumes of final or conditioning waste forms were calculated. Based on given information, unprocessed wastes were roughly determined backward from the waste volume reduction ratio provided in the report and volume of conditioning waste forms. Using this method, secondary unprocessed waste type and volume were correspondingly assigned to the IWMS predefined waste categories (as seen in Table 3-7). Table 3-7 gives details for the secondary waste considered in PUREX process (adjusted COEX process). Since this information for other advanced separation processes (UREX, COEX, FPEX, and etc.) does not exist, those processes were also assumed to possess similar types and amount of secondary wastes as does the PUREX process. For activity fractions, the amounts of radioactivity distributed between various types of secondary wastes produced were assumed to be the same as the volume fractions of the same waste unless specific data can be reasonably obtained either directly or indirectly from literature. Density data were also estimated since actual data usually requires a specific type of waste material.

Table 3-7 Secondary waste generated by adjusted COEX (PUREX) process

Waste type	Volume*(L/kgUO2)	Density(kg/L)	Activity fraction*
COEXMetal	0.0000E+00	7.8740E+00	0.0000E+00
COEXLiq_Aq	3.5787E-02	1.0000E+00	8.0000E-01
COEXLiq_Or	1.5284E-02	7.5000E-01	1.0000E-01
COEXSludge	0.0000E+00	2.0000E+00	0.0000E+00
COEXResin	0.0000E+00	7.0000E-01	0.0000E+00
COEXFilter	5.4233E-01	1.6400E+00	2.0000E-02
COEXTech	5.4233E-01	3.0000E+00	4.0000E-02
COEXEquip	5.4233E-01	1.2300E+00	4.0000E-02
COEXAsh	0.0000E+00	1.5000E+00	0.0000E+00
COEXMixed	0.0000E+00	1.0000E+00	0.0000E+00
COEXMisc1	0.0000E+00	1.0000E+00	0.0000E+00
COEXMisc2	0.0000E+00	1.0000E+00	0.0000E+00

* This fraction has to be summed up to 1.0 for conservation of radioactivity assumption

3.5.1.5 Input parameters in spreadsheet "Wasteforms"

This sheet contains details for waste form development, i.e. manufacturing costs of relevant waste form materials (glass, ceramics, metal, concrete, and polymer); percent waste loading for these materials; volume reduction of various wastes (Dry Active Waste (DAW), liquid waste, wet solid waste and metal waste); and disposal costs for different waste classifications.

3.5.1.6 Input parameters in spreadsheet "HeadendParameters"

Details on head-end processes are located in this spreadsheet. Table 3-8, Table 3-9 and Table 3-10 give the process parameters for chopping, voloxidation and dissolution processes respectively. For the chopping process, required parameters include total fission gas volume (L/MTU), fission gas volumetric released fraction during the process, radioactivity fraction that contributes to secondary wastes and radioactivity fraction that contributes to metal scrap. The last two parameters were assumed to be zero as explained in section 3.5.1.4. Typical fission gases generally contain hydrogen, carbon, krypton, and iodine. The total volume of the fission gas of 1.96218 L/MTU was calculated from a basis given in [79] and burnup of 28.152 MWD/assembly for the Turkey Point 3 UF. Fission gas released during the chopping process was assumed to be 30% of the total fission gas available in the fuel. The rest of the fission gas was assumed to be released during either voloxidation or dissolution depending on the reprocessing scheme specified. By assuming that the fission gas homogeneously distributes throughout the UF, radionuclides released fractions were also assumed to be the same as the volumetric released fraction.

Table 3-8 Chopping process parameters

Nuclide	Fission gas released fractions
H3	3.00E-01
C14	3.00E-01
Kr85	3.00E-01
I129	3.00E-01
F_SW	0.00E+00
F_FP_Vol	3.00E-01
F_SCP	0.00E+00

The voloxidation process requires similar parameters to those required in the chopping process. The volatile radionuclide, which is in gaseous form in nature (shown in Table 3-8), is typically released in the whole amount during voloxidation or dissolution. Semi-volatile radionuclides (shown in Table 3-9) can be released during the voloxidation process but not the dissolution process. The fractions for these semi-volatile radionuclide were obtained from [13 ,80].

Table 3-9 Voloxidation process parameters

Element	Fission gas release fractions
H3	1.00E+00
C14	1.00E+00
Kr85	1.00E+00
I129	1.00E+00
Cs	9.80E-01
Tc	9.23E-01
Ru	9.76E-01
Rh	8.27E-01
Te	5.33E-01
Mo	6.17E-01
F_FP_Vol	7.00E-01
F_SW	1.00E-07

The dissolution process requires not only the parameters required by chopping process but also radionuclides distribution across all the products, such as dissolved radionuclides in nitric acid solution, in empty fuel cladding (empty hulls) and in non-dissolved solids. The dissolution experiment using an actual UF was performed [15]. Although the UF used in the experiment was not the same as the UF used in the IWMS modeling, the parameters obtained from this experiment were considered reasonable. The fission gas that is not released during the chopping process was assumed to be released during the dissolution process hence the release fraction of 1.0 was used as shown in Table 3-10.

Table 3-10 Dissolution process parameters

Dissolution Process Parameters (DISS1_BOX.INP)		Dissolution (of chopped fuel) Process Parameters (DISS2_BOX.INP)			
Nuclide	**Fission gas release fractions**	**Element**	**Dissolution**	**Non-Dissolved**	**In cladding**
H3	1.00E+00	Rb	0.9950	0.0030	0.0020
C14	1.00E+00	Sr	0.9840	0.0090	0.0070
Kr85	1.00E+00	Y	0.9740	0.0160	0.0100
I129	1.00E+00	Zr	0.0020	0.0060	0.9920
Dissolution Process Parameters (DISS1_BOX.INP)		**Dissolution (of chopped fuel) Process Parameters (DISS2_BOX.INP)**			
Fission gas release fractions		**Element efficiency**			
Nuclide	**fraction**	**Element**	**Dissolution**	**Non-Dissolved**	**In cladding**
F_FP_Vol	7.00E-01	Mo	0.1320	0.8490	0.0190
F_SW	1.00E-07	Tc	0.9140	0.0620	0.0240
Cost_HNO3	2.33E+02	Ru	0.9850	0.0120	0.0030
		Rh	0.9930	0.0050	0.0020
		Pd	0.3630	0.0060	0.6310
		Ag	0.0250	0.6140	0.3610
		Cd	0.1570	0.0280	0.8150
		Sn	0.0200	0.1090	0.8710
		Te	0.4350	0.5210	0.0440
		Cs	0.9750	0.0050	0.0100
		Ba	0.9370	0.0170	0.0460
		La	0.9810	0.0000	0.0190
		Ce	0.9990	0.0000	0.0010
		Nd	0.9990	0.0000	0.0010
		Eu	0.9990	0.0000	0.0010
		Gd	1.0000	0.0000	0.0000
		U	1.0000	0.0000	0.0000
		Np	0.9980	0.0020	0.0000
		Pu	0.7960	0.1980	0.0060
		Am	1.0000	0.0000	0.0000

3.5.1.7 Input parameters in spreadsheet "SeparationParameters"

Details on the separation processes are located in this spreadsheet. Parameters required in this section are (1) the volumetric flow rate ratios for all incoming streams to initial feed, (2) the distribution of radionuclides of interest to a given process (i.e. U and Tc for the UREX process; Cs and Sr for the FPEX process) across all product streams (direct, indirect and secondary waste streams), and unit cost (USD/L) of all raw material streams. Table 3-11 gives an example of the details of the UREX process parameters. Flow parameters were obtained from [17] .Similar information is also required for other separation processes such as FPEX, TRUEX and etc.

Table 3-11 UREX process parameters

UREX flow parameters (UREX_BOX.INP)		
Description	**Variable name**	**(L/L Aq.feed)**
Volume ratio of minimum required TBP	Vol_TBP	1.05E+00
Volume ratio of minimum required Dodecane	Vol_Dod	2.46E+00
Volume ratio of 0.3 M HNO3 scrub	Vol_Dscr_HNO3	5.79E-01
Volume ratio of 0.01 M HNO3 U strip	Vol_Dstr_HNO3	3.51E+00
Volume ratio of 6.0 M HNO3 Tc strip	Vol_Hstr_HNO3	9.65E-01
Volume ratio of diluted HNO3 Wash solution	Vol_Dwas_HNO3	1.50E+00
UREX flow parameters (UREX_BOX.INP)		
Description	**Variable name**	**(L/L Aq.feed)**
Volume ratio of AHA	Vol_AHA	4.70E-01
U Fraction distributed in wash effluent*	WASH_EFF_U	5.00E-07
Tc Fraction distributed in wash effluent*	WASH_EFF_Tc	5.00E-07
U Fraction distributed in spent solvent	SPNT_EFF_U	1.00E-06
Tc Fraction distributed in spent solvent	SPNT_EFF_Tc	1.00E-06
Fraction of activity subjected to contribute to SW*	F_SW	1.00E-07
Fraction of activity subjected to contribute to solvent(not U and Tc)	F_SOLV	1.00E-06
Unit cost for UREX raw materials	**Variable name**	**(USD/L)**
30% TBP	Cost_TBP	3.80E+01
70% Dodecane	Cost_Dod	2.53E+04
1.0 M HNO3 Feed	Cost_HNO3	8.32E+00
0.01 M HNO3 U strip	Cost_HNO3	8.32E-02
6.0 M HNO3 Tc strip	Cost_HNO3	4.99E+01
1.0 M HNO3 Wash solution	Cost_HNO3	8.32E-02
0.47 M AHA	Cost_AHA	4.15E+02

3.5.1.8 Input parameters in spreadsheet "SupportParameters"

Details on the support processes are located in this spreadsheet. Similar information to that needed in separation process input parameter section is also required for all the support processes such as off-gas treatment, MOX fuel fabrication and next generation fuel fabrication processes. Table 3-12 gives an example of the details of the off-gas treatment process parameters [39 ,40 ,42 ,81]. For MOX fuel fabrication, the process parameters were obtained from Reference [35 ,36 ,82]. Process parameters for the next generation fuel fabrication process were assumed based on the current MOX fuel fabrication process due to a limitation in data availability.

Table 3-12 Off-gas treatment process parameters

Description	Variable name	Volume (L/L FP gas)
Volume of raw material number 1 (Lrawmat1/L Fpgas)	Vol_Rawmat1	3.00E-01
Volume of raw material number 2 (Lrawmat2/L Fpgas)	Vol_Rawmat2	7.00E-01
Volume of raw material number 3 (Lrawmat1/L Fpgas)	Vol_Rawmat3	1.00E+00
Volume of raw material number 4 (Lrawmat2/L Fpgas)	Vol_Rawmat4	1.00E+00
Volume of raw material number 5 (Lrawmat1/L Fpgas)	Vol_Rawmat5	1.00E+00
Volume of raw material number 6 (Lrawmat2/L Fpgas)	Vol_Rawmat6	1.00E+00
Volume of C-14 product{adsorbent} (L C14/L Fpgas)	Vol_C14	9.80E-01
Volume of H-3 product (L H3/L Fpgas)	Vol_H3	8.30E-01
Volume of Kr-85 product produced per unit gas input (L Kr85/L Fpgas)	Vol_Kr85	9.80E-01
Volume of I-129 product produced per unit gas input (L I129/L Fpgas)	Vol_I129	9.80E-01
Volume of Cs product produced per unit gas input (L Cs/L Fpgas)	Vol_Cs	9.80E-01
Volume of Tc product produced per unit gas input (L Tc/L Fpgas)	Vol_Tc	9.80E-01
C-14 decontamination efficiency	Dect_Eff_C14	9.90E-01
H-3 decontamination efficiency	Dect_Eff_H3	9.90E-01
Kr-85 decontamination efficiency	Dect_Eff_Kr85	9.90E-01
I-129 decontamination efficiency	Dect_Eff_I129	9.90E-01
Cs decontamination efficiency	Dect_Eff_Cs	9.90E-01
Tc decontamination efficiency	Dect_Eff_Tc	9.90E-01
Fraction of activity subjected to contribute to SW	F_SW	1.00E-06
raw material number 1 (Lrawmat1/L Fpgas)	Cost_Rawmat1	3.00E-01
raw material number 2 (Lrawmat2/L Fpgas)	Cost_Rawmat2	7.00E-01
raw material number 3 (Lrawmat1/L Fpgas)	Cost_Rawmat3	1.00E+00
raw material number 4 (Lrawmat2/L Fpgas)	Cost_Rawmat4	1.00E+00
raw material number 5 (Lrawmat1/L Fpgas)	Cost_Rawmat5	1.00E+00
raw material number 6 (Lrawmat2/L Fpgas)	Cost_Rawmat6	1.00E+00

3.5.1.9 Input parameters in spreadsheet "GroundWaterTransport"

Parameters related to groundwater transport with large uncertainty are located in this spreadsheet. Information in this spreadsheet is for the calculation of Committed Effective Dose Equivalent (CEDE) at the disposal site exclusion zone boundary at 10000 years after disposal. Table 3-13 shows the parameters for the Yucca Mountain facility [83-86]. Distribution coefficients for some of the elements listed in Table 3-13 are not available, hence they were assumed to be the same as other elements having similar chemical properties. Similar information is also required for the mixed low level waste facility at Texas for both unsaturated and saturated zones. Information for this facility was taken from the application for a license to authorize near-surface land disposal of low-level radioactive waste[ff].

Table 3-13 Groundwater Transport parameters for Yucca Mountain Facilities

Parameter	Variable	Value
Hydraulic conductivity of the aquifer1 (m/yr)	Hyd_Cond	4.38E+03
Effective porosity	Eff_Porosity	1.80E-01
Bulk density (g/cm^3)	Bulk	1.27E+00
Distribution coefficient k_d (mL/g) for		
Ac	Kd_Ac	1.05E+03
Ag	Kd_Ag	3.00E+02
Am	Kd_Am	1.05E+03
Ba	Kd_Ba	3.00E+02
Bi	Kd_Bi	3.00E+02
Bk	Kd_Bk	3.00E+02
C	Kd_C	0.00E+00
Cd	Kd_Cd	3.00E+02
Ce	Kd_Ce	3.00E+02
Cf	Kd_Cf	3.00E+02
Cl	Kd_Cl	0.00E+00
Cm	Kd_Cm	1.05E+03
Co	Kd_Co	3.00E+02
Cs	Kd_Cs	2.51E+03
Eu	Kd_Eu	3.00E+02
Fe	Kd_Fe	3.00E+02
H	Kd_H	3.00E+02
He	Kd_He	3.00E+02
Ho	Kd_Ho	3.00E+02
I	Kd_I	0.00E+00
Kr	Kd_Kr	3.00E+02
Mn	Kd_Mn	3.00E+02
Mo	Kd_Mo	3.00E+02
Nb	Kd_Nb	1.05E+03
Ni	Kd_Ni	2.50E+02
Np	Kd_Np	7.50E+00
Pa	Kd_Pa	5.00E+01
Pb	Kd_Pb	3.00E+02
Pd	Kd_Pd	2.50E+02
Pm	Kd_Pm	3.00E+02
Pu	Kd_Pu	1.75E+02
Ra	Kd_Ra	2.55E+03
Rh	Kd_Rh	3.00E+02
Ru	Kd_Ru	3.00E+02
Sb	Kd_Sb	3.00E+02
Se	Kd_Se	1.50E+01
Sm	Kd_Sm	1.05E+03
Sn	Kd_Sn	1.60E+02
Sr	Kd_Sr	2.50E+04
Tc	Kd_Tc	0.00E+00
Te	Kd_Te	3.00E+02

[ff] http://www.urs-slc.com/wcs/

Table 3-13 Continued

Parameter	Variable	Value
Distribution coefficient k_d (mL/g) for		
Th	Kd_Th	1.05E+03
U	Kd_U	1.00E+01
V	Kd_V	3.00E+02
Y	Kd_Y	3.00E+02
Zr	Kd_Zr	1.05E+03

3.5.1.10 Input parameters in spreadsheet "Top_level"

The "top_level" spreadsheet contains a table where the relative importance between top-level decision criteria can be supplied by users. The importance matrix, which can be constructed from the user-specified relative importance, is used to calculate the decision weights. The Visual Basic for Application (VBA) is executed: 1) to export the weights matrix to the MATLAB, 2) to run the MATLAB application and 3) to import an eigenvector back into the spreadsheet. The MATLAB software is utilized to solve for the real eigenvalue and its corresponding eigenvector of the importance matrix (a matrix of this type has only one real eigenvalue). The weights of the decision criteria can be obtained from the eigenvector previously mentioned. The resulting weights are also displayed in the same spreadsheet, exported in the same manner as other parameters on other spreadsheets, and made available for the main FORTRAN code when needed.

3.5.1.11 Input parameters in spreadsheet "Sub_level"

The "sub_level" spreadsheet contains the same type of information as does the "top-level" except for the list of decision criteria.

3.5.2 IWMS Output Parameters

All output files are also written in text file format (*.out). To save the calculation time, only the results that are most important to overall waste management strategy selection (e.g. radiation doses, cost and volume of final waste forms) are imported back into a MS Excel spreadsheet named “IWMS-AFC”. These results are given in Table 3-14, Table 3-15, Table 3-16 and Table 3-17. Table 3-14 shows the cost summary of the specified reprocessing scheme. Table 3-15 and Table 3-16 show waste volume summaries. Table 3-17 shows global output from IWMS code. Rows with filled numbers shown in Table 3-14 and 3-15 correspond to the calculated results for the processes chosen at the beginning of the calculation, while blank cells simply mean those processes were not chosen as part of the reprocessing scheme.

Table 3-14 Reprocessing and stream management costs by process (USD/MTU)

Process Code	Operation Maintenance	Raw Materials	Capital	Decommissioning	Separation total	Stream Management total	Total
DISB	2.070E+03	0.000E+00	3.450E+04	9.802E+02	3.755E+04	8.728E+01	3.764E+04
CHOP	2.070E+03	0.000E+00	3.450E+04	9.802E+02	3.755E+04	0.000E+00	3.755E+04
VOLX							
DISSC	2.070E+03	1.092E+05	3.450E+04	9.802E+02	1.468E+05	1.655E+04	1.633E+05
DISSV							
UREX							
COEX	2.070E+03	6.849E+03	3.450E+04	9.802E+02	4.440E+04	3.984E+05	4.428E+05
FPEX							
CCDPEG							
TRUEX							
TALSPEAK							
REVTAL							
MOXFUEL	1.000E+03	1.923E+03	1.667E+03	9.293E+03	1.388E+04	0.000E+00	1.388E+04
NEXFUEL							
OFGTC	2.070E+03	4.050E+00	3.450E+04	9.802E+02	3.756E+04	2.852E+02	3.784E+04
OFGTV							
Total	1.135E+04	1.180E+05	1.742E+05	1.419E+04	3.177E+05	4.153E+05	7.330E+05

Table 3-15 Volume of final waste form of direct waste streams from UREX (L)

Process Code	A	B	C	GTCCLW	GTCCHW	TRU	MLLW	Total
DISB	0.000E+00	0.000E+00	0.000E+00	0.000E+00	4.475E+00	0.000E+00	0.000E+00	4.475E+00
CHOP	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
VOLX								0.000E+00
DISSC	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	1.759E+02	0.000E+00	1.759E+02
DISSV								0.000E+00
UREX								0.000E+00
COEX	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	1.910E+05	0.000E+00	1.910E+05
FPEX								0.000E+00
CCDPEG								0.000E+00
TRUEX								0.000E+00
TALSPEAK								0.000E+00
REVTAL								0.000E+00
MOXFUEL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 3-15 Continued

Process Code	**A**	**B**	**C**	**GTCCLW**	**GTCCHW**	**TRU**	**MLLW**	**Total**
NEXFUEL								0.000E+00
OFGTC	0.000E+00	1.406E+01	7.615E+00	7.615E+00	0.000E+00	0.000E+00	0.000E+00	2.929E+01
OFGTV								0.000E+00
Total	0.000E+00	1.406E+01	7.615E+00	7.615E+00	4.475E+00	1.912E+05	0.000E+00	1.913E+05

Table 3-16 Volume of final waste form of secondary waste streams from UREX (L)

Waste Type	**A**	**B**	**C**	**GTCCLW**	**GTCCHW**	**TRU**	**MLLW**	**Total**
Metal	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Liq_Aq	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.426E+03	0.000E+00	2.426E+03
Liq_Or	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	7.755E+02	0.000E+00	7.755E+02
Sludge	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Resin	3.924E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	3.924E+01
Filter	9.173E+03	0.000E+00	4.257E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	9.177E+03
Tech	2.293E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.293E+03
Equip	9.177E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	7.701E+02	0.000E+00	9.947E+03
Ash	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Mixed	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	4.709E+01	4.709E+01
Misc1	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Misc2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Total	2.068E+04	0.000E+00	4.257E+00	0.000E+00	0.000E+00	3.971E+03	4.709E+01	2.471E+04

Table 3-17 Global IWMS output

Output parameters from selected reprocessing scheme	
Average Committed Effective Dose Equivalent (mrem/y)	1.018112E-03
Total Cost of reprocessing (USD/MTHM)	2.270951E+08
Total Volume of HLW (m^3)	5.507690E-04
Total Volume of LLW (m^3)	1.449822E+00
Total Volume of TRU (m^3)	3.859112E+00
Total Volume of MLLW (m^3)	3.628890E+00
Figure of Merit (Max among all streams)	1.344469E-01
Mode Committed Effective Dose Equivalent (mrem/y)	0.000000E+00
Maximum Committed Effective Dose Equivalent (mrem/y)	2.833630E-02

3.6 Model Validation and Benchmarking

In order to ensure the validity of the code, comparison between IWMS calculation results and actual data is essential. It is unreasonable to compare all aspects of the IWMS calculated results with the actual information simply because most of the information is unavailable to the public and in some cases does not exist. A reasonable benchmarking approach was done in two parts: (1) comparison of the ratio of the concentration (of key elements) after the separation process to the one before separation and (2) comparison of final conditioned waste volume. The purpose of the first and the second parts were to verify separation efficiency and radionuclide mass balance calculation, and to compare the relevant waste treatment and conditioning calculation, respectively. Due to the availability of the resources, two sets of mass balance comparisons were performed for the UREX and PUREX processes and one set of waste volume comparison was performed for the PUREX process because no information regarding waste generation exists for the UREX process. Because the IWMS adopts the UREX+ as a baseline process, the PUREX process is not part of this IWMS scheme. Instead, the adjusted COEX process was used as a representative for the PUREX process in the benchmarking. Only deterministic calculation was performed in benchmarking process. Once the comparison process was completed, case studies were performed in a probabilistic manner. This required most of the input parameters to change according to their probability density characteristics.

3.6.1 Mass balance comparisons

3.6.1.1 UREX mass balance comparisons

The UREX flowsheet that was used for benchmarking is shown in Figure 3-14[16]. The flow rate parameters also served as a basis for the rest of the UREX process parameters. The goals of the UREX demonstration were to: (1) recover greater than 99.9 % of U in the U product stream, (2) recover greater than 95.0% of Tc in Tc product stream and (3) retain greater than 99.9% of TRU isotopes in the raffinate stream.

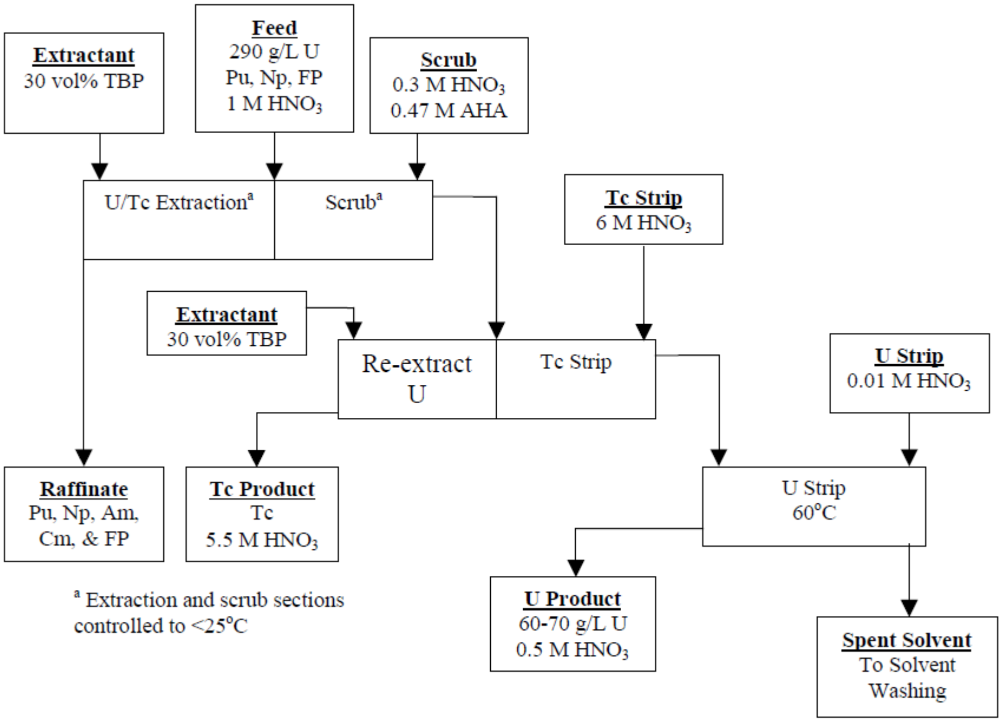


Figure 3-14 UREX process flow sheet

All three tests were performed successfully with Dresden fuel solution. The analytical results from the test number 2 are given in Table 3-18.

Table 3-18 Test #2 results concentration of key elements in the UREX streams

Key element	U-product stream	Tc-product stream	Raffinate
U	> 99.9%	0.0001%	0.016%
Tc	NA	> 95.0%	NA
Pu	0.011%		> 99.9%

The UF from the Turkey Point reactor was used in the all reprocessing scheme not only for the benchmarking calculation but also the rest of the case studies throughout this research. The initial mass of key radionuclides in the initial feed can be found in the output file named either “diss_check1.out” or “UREX_check1.out”. In the first file, one should look for mass information in the product stream section and in the second file one should look for mass information in the raw material stream section. All masses of the radionuclides of the same element were summed to get the total mass of that element. These calculations from IWMS modeling are given in Table 3-19. The information shown in Table 3-19 is used to calculate the percentage of mass balance of key elements, shown in Table 3-19. Table 3-19 also shows the comparison between test# 2 and IWMS results.

Table 3-19 Mass balance calculations of key elements from UREX under IWMS

Key element	Mass of the element distributed in main stream (kg)			
	Initial feed	U-product UREXT1P1	Tc-product UREXT2P1	Raffinate UREXT1P2
U	9.8101E+02	9.8091E+02	0	9.7610E-02
Tc	3.0317E-01	0	2.4925E-02	6.0630E-03
Pu	4.1069E+00	0	0	4.1069E+00

Table 3-20 IWMS results in comparison with actual UREX hot test

Key element	U-product stream		Tc-product stream		Raffinate	
	Test	UREXT1P1	Test	UREXT2P1	Test	UREXT1P2
U	> 99.9%	99.99%	0.00%	0%	0.02%	0.01%
Tc	NA	0%	> 95.0%	98.000%	NA	2.00%
Pu	0.005%	0%	0.005%	0%	> 99.9%	100.00%

3.6.1.2 PUREX mass balance comparisons

The adjusted COEX process has the following characteristics;

(1) Only U and Pu are co-extracted, i.e. no Np or Tc is separated during the process by setting target separation efficiencies to zero for both elements.

(2) Due to the process resource constraints (either commercially or politically classified), flow parameters (ones that are required in “SeparationParameter” spreadsheet) were reasonably derived from the open literature PUREX closest match process, i.e. the PUREX process designed for Barnwell plant. This plant was never finished hence it was never in operation. The Barnwell PUREX flow sheet is shown in Figure 3-15. Both the flow parameter and the flow diagram were taken from Reference [8]. The goal for the Barnwell plant was to recover at least 98.5 % of U and Pu from the initial feed.

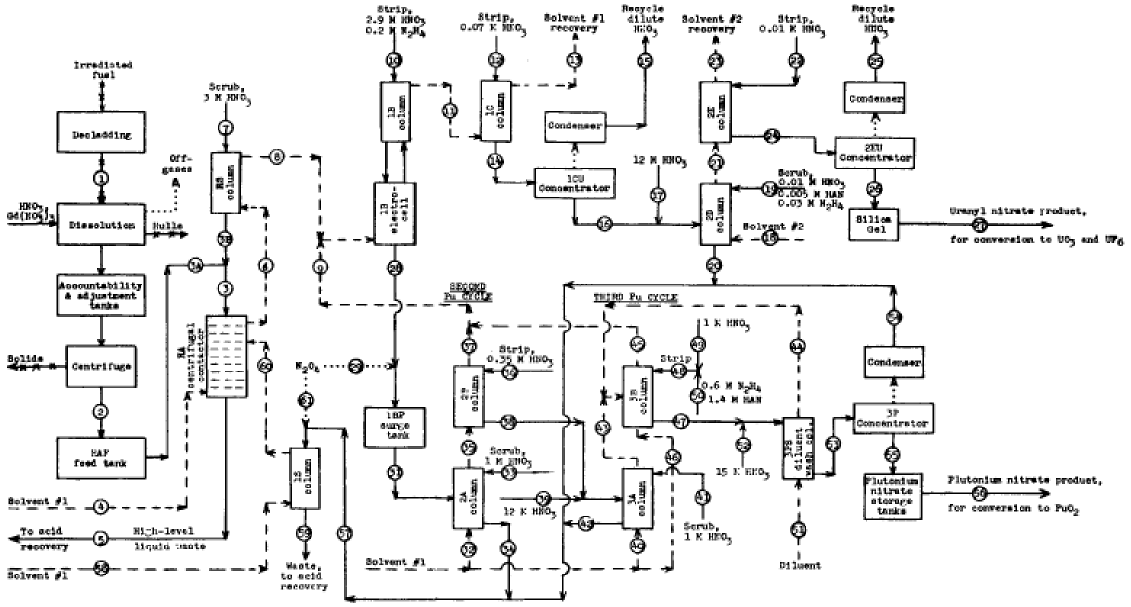


Figure 3-15 Process flow diagram of the PUREX process at Barnwell Plant

The mass distributions of the adjusted COEX process and the comparison results are given in Table 3-21 and Table 3-22, respectively.

Table 3-21 Mass balance of key elements from adjusted COEX under IWMS

Key element	Mass of the element distributed in main stream (kg)			
	Initial feed	U-product COEXT1P1	Pu-product COEXT2P2	Raffinate COEXT1P2
U	9.81006E+02	9.80908E+02	0	9.02525E-02
Pu	4.10687E+00	0	4.10646E+00	3.77832E-04

Table 3-22 IWMS results in comparison with PUREX process at Barnwell plant

Key element	U-product stream		Pu-product stream		Raffinate	
	Barnwell	COEXT1P1	Barnwell	COEXT2P2	Barnwell	COEXT1P2
U	> 98.5%	99.99 %	NA	0	NA	0.00920 %
Pu	NA	0	> 98.5%	99.99 %	NA	0.00920 %

The IWMS results generally agreed with the test results because of the assumption that the mass of the target elements were calculated based on their separation efficiencies. The UREX parameters in IWMS were also obtained from the literature; hence the calculated separation efficiencies strongly agreed. This suggests that the IWMS mass balance calculation schemes are reasonable and valid.

3.6.2 Waste volume comparisons

The waste from the adjusted COEX reprocessing scheme was employed as a basis for comparison for this part. The available literature resource on radioactive waste associated with UF reprocessing can be found from French reprocessing plants archives. The average conditioned waste volumes over the course of plants operations (since startup) were used as a reference for the comparison. Since the French waste definition and classification system differ from the US system, certain assumptions were made. The French system adopted the IAEA waste classification, i.e. LLW, ILW and HLW, while the U.S. system has more refined LLW, a different HLW definition, no ILW, and additional TRU and mixed waste. To be able to compare them, the French wastes remained as they were classified but the IWMS waste had to be slightly adjusted. The combination of all LLWs, i.e. class A, class B and class C LLW; GTCCLW; and MLLW were compared to the French LLW. The combination of GTCCHW and TRU waste were compared to the French HLW. In addition, IWMS took into account the fuel fabrication as part of the reprocessing scheme but the waste volume obtained from the French did not account for such a process, hence all wastes associated with fuel fabrication derived by the IWMS were subtracted before making the comparison. The PUREX waste data was obtained from Reference [87].

For the IWMS to estimate the amount of waste associated with its reprocessing scheme, relevant input parameters, such as unit secondary wastes information (one that is required in "2^{nd}_waste" spreadsheet), are required. Again, the ideal practice would be utilization of the same facility used as a basis for the reprocessing, i.e. using waste generation data from the Barnwell plant which adopted PUREX or waste generation from UREX process. Since the Barnwell plant never operated, there is no unit secondary waste information available, and the UREX process has never been operated in large enough scale to carry the waste generation data. To fill this required input parameter, the data was translated and derived from the French reprocessing waste treatment facility at La Hague[78]. It is unfortunate that the PUREX process flow data is not available. Otherwise it would be best to use all the relevant data from the same French facility. The document described the major waste from the facility in term of the total inventory (i.e. without specific detail on where each type of the wastes originated), as well as their treatment methodologies. The waste type included high and low level liquid wastes; and solid waste, which in the document was referred to as process waste and plant waste. These wastes were assumed to equally: (1) distribute across the waste types and (2) result from the process segments employed. The reprocessing scheme employed was assumed to include all head-end process with the exception of voloxidation, PUREX, off-gas treatment (Most of the effluent gas was released from that facility, hence very little waste from off-gas treatment process was assumed from the document) and no fuel fabrication process. The waste associated with fuel fabrication process was subtracted from the total IWMS waste before making a comparison. The comparison results are given in Table 3-23.

Table 3-23 Comparison of conditioned waste volume of waste derived from PUREX process and IWMS estimated (m^3/MTHM)

Waste type	IWMS	PUREX
LLW	4.489E+00	4.502E+00
HLW	6.909E-01	1.800E-01

Due to the nature of the problem of this type, possible explanations for the differences observed in Table 3-23 include:

(1) The difference in waste definitions and classification system between the French and the U.S. system.

(2) The assumption of flow parameters that could affect a direct waste from the process.

(3) The assumption on the unit secondary waste distribution across the waste types and the employed processes.

(4) The uncertainty in waste volume reduction ratio for various types of wastes treatment and conditioning technologies. This factor when combined with the uncertainty in waste definition could lead to quite large effects.

(5) The time independent assumption, i.e. the steady state assumption, of all the relevant processes could be one of the possible reasons. In IWMS, steady state conditions were assumed for all the employed processes. The relevant parameters used in the calculation of final waste volume (such as volumetric flow rate of waste streams) were approximated at the highest process throughputs. For the PUREX process, representative waste volume was the average of the conditioned waste volume over the operation time since the beginning of its operation.

(6) The assumption on the radioactivity contribution to secondary waste streams could also explain the differences. Although expert judgment and reprocessing plant personnel agree that this secondary waste does vary a little by the initial radionuclide inventory of the incoming UF, the exact fraction has never been revealed because industrial scale has a tendency to focus on the overall effect rather than a specific point. However, in practice this fraction does depend on the initial inventory of the UF so it was incorporated as part of the IWMS modeling. Hence in this research, this fraction (for all process segments), again, was assumed. As a result, it could contribute the difference as previously seen.

3.6.3 Bateman Equation Approximation

To verify the correctness of the code for the Bateman approximation part, selected IWMS calculated nuclide concentrations were compared with hand calculated ones, i.e. certain nuclides that belong to decay chain number 1 and decay chain number 5 were compared. Both set of results matched exactly as seen in Figure 3-16 and Figure 3-17.

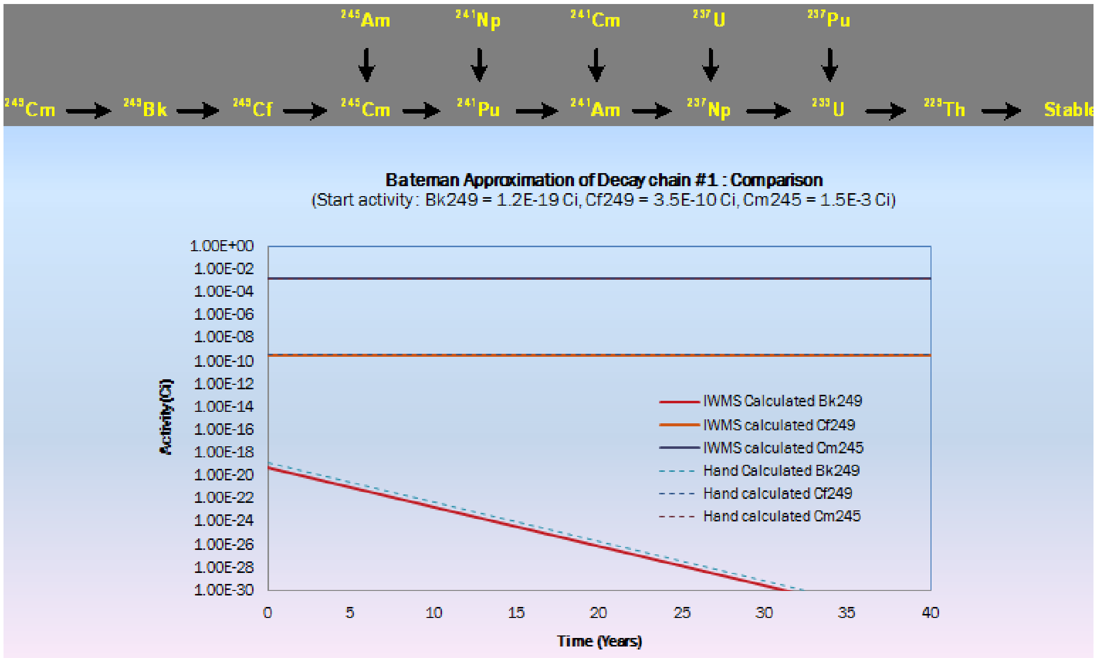


Figure 3-16 Bateman Approximation of Decay chain #1: Comparison with hand calculation

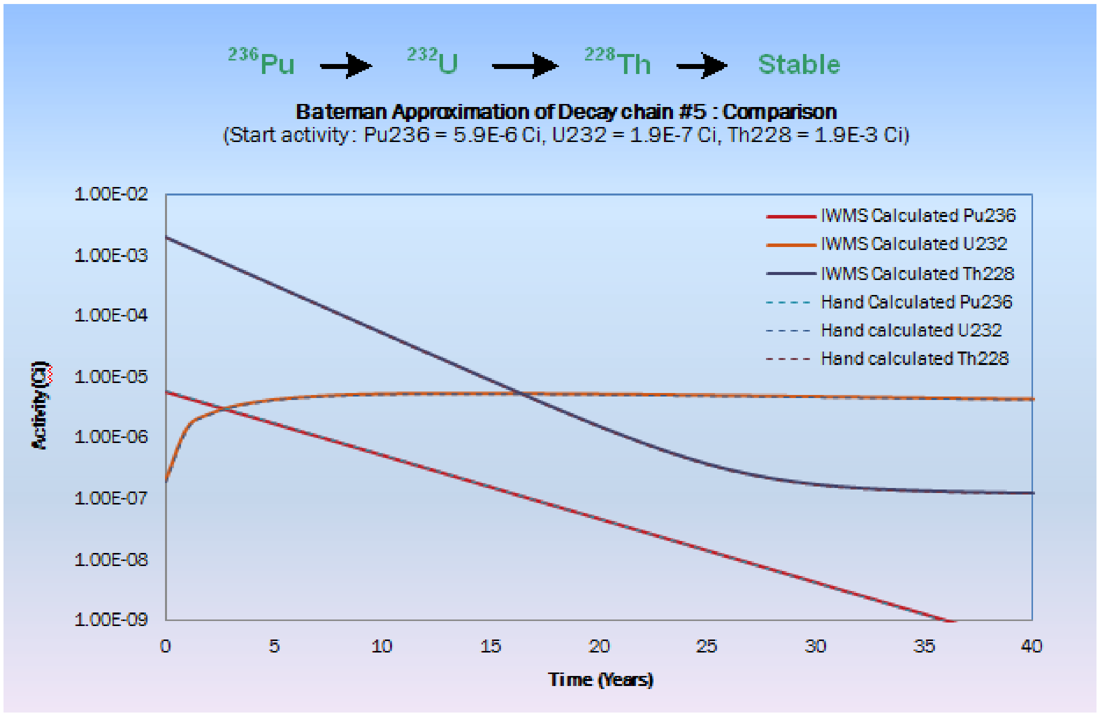


Figure 3-17 Bateman Approximation of Decay chain #5: Comparison with hand calculation

3.6.4 Unsaturated zone transport model

To verify the unsaturated zone transport model, the sample waste stream was used. Figure 3-18 illustrates how both of the unsaturated and saturated zone transport models were individually tested.

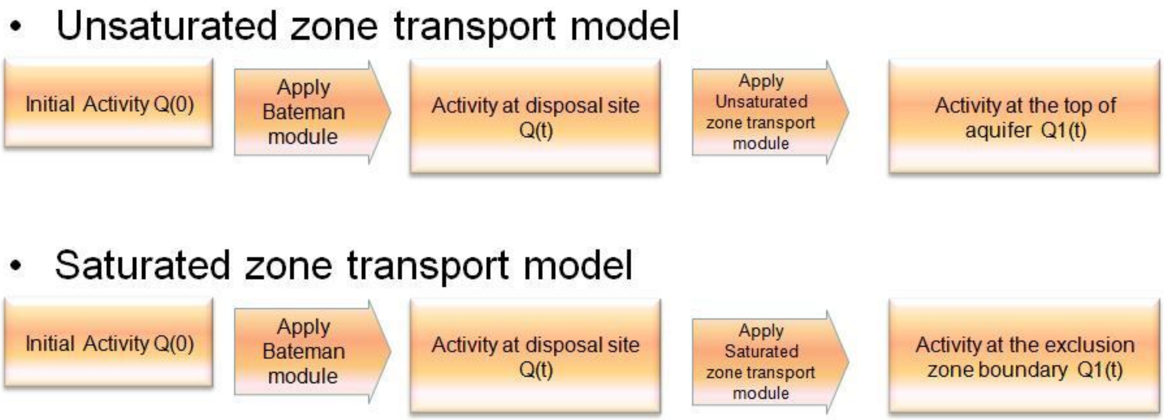


Figure 3-18 Groundwater Transport Model Verification Diagram

Calculation results from the IWMS code were compared with hand calculations; and were identical for all the nuclides transported through the unsaturated zone. The selected results are given in Table 3-24. Table 3-25 shows input parameters used in the calculation. They were obtained from the waste disposal site in Andrews County, Texas.

Table 3-24 Unsaturated zone transport calculation results

Nuclide	Transit time to aquifer (y)	Retardation factor
C14	2.00E+10	1.00E+00
Cl36	3.67E+10	1.84E+00
H3	2.00E+10	1.00E+00
He4	2.00E+10	1.00E+00
I129	3.67E+10	1.84E+00
Np237	8.58E+11	4.30E+01
Se79	3.89E+11	1.95E+01
Tc98	3.67E+10	1.84E+00
Tc99	3.67E+10	1.84E+00
U238	8.40E+12	4.21E+02

Table 3-25 Input parameters used in unsaturated zone model verification

Input parameters	Values
Depth to the aquifer(m)	9.0000E+01
Percolation Rate ($\frac{m}{y}$)	1.1938E-03
Volumetric water content in the unsaturated zone ($\frac{m^3}{m^3}$)	4.8900E-02
Bulk density ($\frac{g}{m^3}$)	1.6800E+00
Porosity	2.0000E-01

3.6.5 Saturated zone transport model

IWMS saturated zone transport calculation results using the approach shown in Figure 3-18 were compared to hand calculation. Based on the model used (Equation 3-15), the ϑ term, time shift term and exponential terms were hand calculated. These numbers are displayed in the table located in Figure 3-19. For verification purposes, only radioactivity of Np-237 at the disposal site and its boundary were calculated using IWMS model and the results were also plotted in Figure 3-19. The plots demonstrated that both activities reach the saturation level. By looking at the Equation 3-15, there are three characteristic factors: (1) the ϑ term, (2) the scaling exponential term and (3) the time shift term. By comparing the plot of the activity at the disposal site boundary with hand calculations, both ϑ and scaling exponential terms were matched. Both the plot and the numbers in the table indicated that they were closed to unity. The time shift term (the time when the activity at site boundary started to rise) was about 2600 years from the plot, and matched the 2657 years indicated in the hand calculated table. Input parameters used in these calculations are given in Table 3-26.

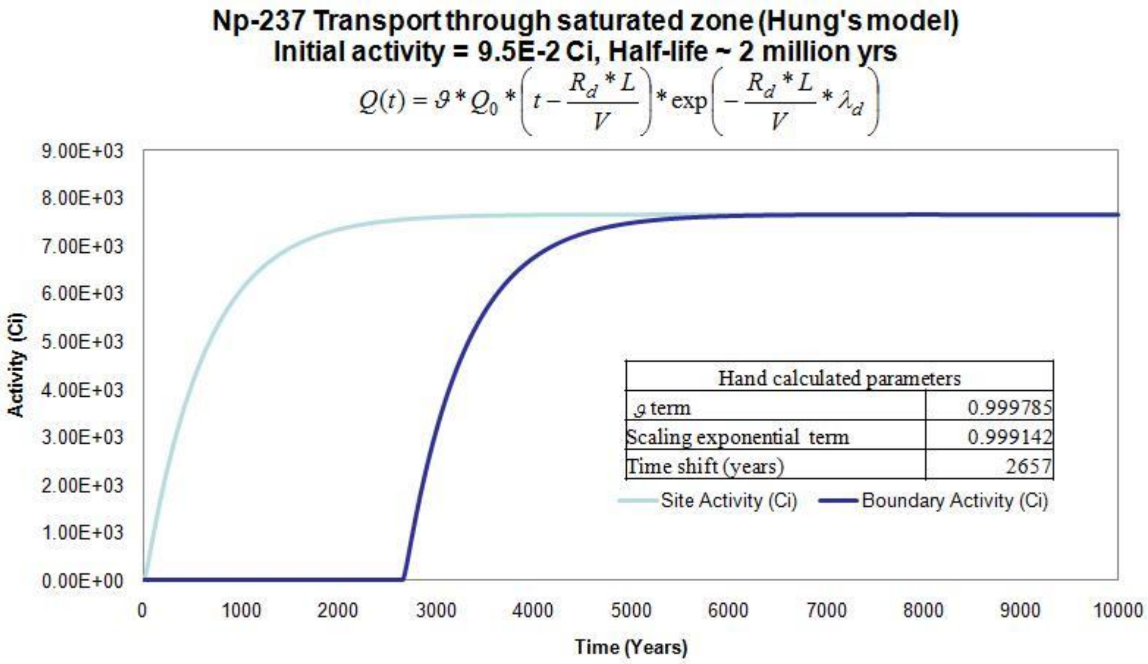


Figure 3-19 IWMS calculated activity of Np-237

Table 3-26 Input parameters used in saturated zone model verification

Input parameters	Values (For Np-237)
Retardation factor	5.39167E+01
Diffusion coefficient ($\frac{m^2}{s}$)	1.09350E-01
Peclet number	6.01235E+07
Site porosity	1.80000E-01
Site effective porosity	1.80000E-01
Site boundary (m)	1.80000E+04
Site hydraulic conductivity ($\frac{m}{y}$)	4.38300E+03
Bulk density ($\frac{g}{m^3}$)	1.27000E+00
Interstitial velocity ($\frac{m}{y}$)	3.65250E+02
Decay constant(per year)	3.23225E-07
Velocity of nuclide in fluid ($\frac{m}{y}$)	3.65250E+02
Distribution coefficient ($\frac{mg}{L}$)	7.50000E+00

Chapter 4 Case Studies and Discussions

To demonstrate the application of the IWMS code, the UREX process was used as a case study since it is the only separation process that has been tested and whose results were publicly available. To apply the UREX process, certain necessary head-end and support processes are needed. These include fuel disassembling, chopping, and dissolution processes for head-end part, and off-gas treatment and mixed-oxide fuel fabrication processes for support processes. Please note that the voloxidation process was not employed as part of the head-end in this case study because the tested UREX process has not been verified with voloxidation process incorporated. A schematic diagram for this UREX process is shown in Figure 4.1.

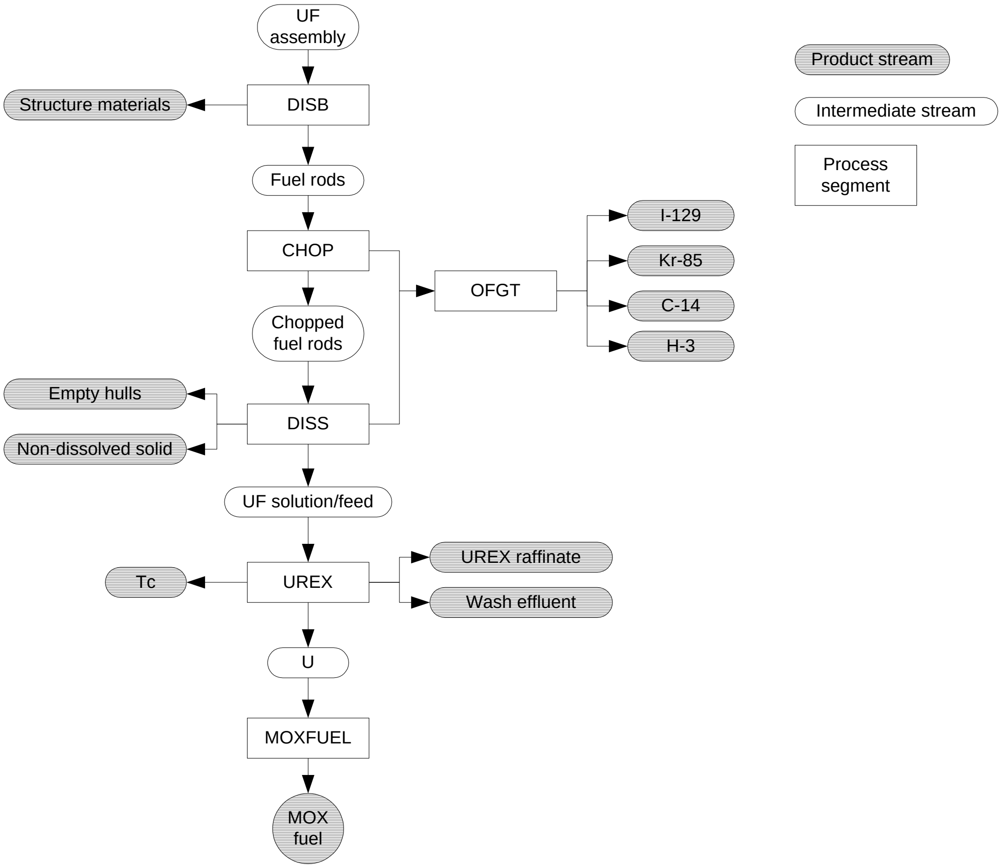


Figure 4-1 Process flow diagram of UREX process in IWMS case study

4.1 Case study input parameters

As indicated earlier, UREX was specified as a desired reprocessing scheme, with a target separation efficiency of 99.99 and 98.00 percent for U and Tc, respectively. The used fuel used in this case study was the fuel discharged from Turkey Point 3 reactor. The irradiation history of this fuel was provided by the US NRC (NUREG/CR-0200). This information was used as ORIGEN-ARP input parameters to generate the radionuclide inventories used as one of the IWMS inputs. These inventories are given in Appendix F. Other required input parameters are explained in the previous chapter with some details given in corresponding appendices mentioned earlier.

4.2 Sensitivity study on the UREX case study

Most of the IWMS input parameters are unavailable, hard to find or uncertain in nature, hence sensitivity analyses were performed first to identify the most sensitive input parameters to the IWMS final output. In this case study, the two global output parameters used as an indicator for effective waste management are the total cost and the average committed effective dose equivalent (across various waste streams) at 10000 years post disposal. Because IWMS modeling involves a sizable number of input parameters even for the sensitivity analysis (on the order of several hundred input parameters), only screened input parameters were included in this sensitivity study. The totals of 237 out of 500 plus input parameters were studied. They are grouped and listed below. The numbers in parentheses are the actual number of input parameters being studied.

- Secondary waste unit generation parameters (9)
- Waste form manufacturing parameters, i.e. VR, waste loading (9)
- Cost parameters, i.e. reprocessing, waste handling, waste disposal costs (25)
- Groundwater transport parameters, i.e. sorption coefficient (184), Hydraulic conductivity (2), groundwater discharge (2), percolation rate (2), bulk density (2), porosity (2)

Sensitivity studies were performed by increasing and decreasing one input parameter from its based value while keeping other input parameters constant. The global outputs were observed for each input parameter changed. Figure 4-2 and Figure 4-3 show the sensitivity charts (of the most sensitive parameters) for the total cost and CEDE respectively.

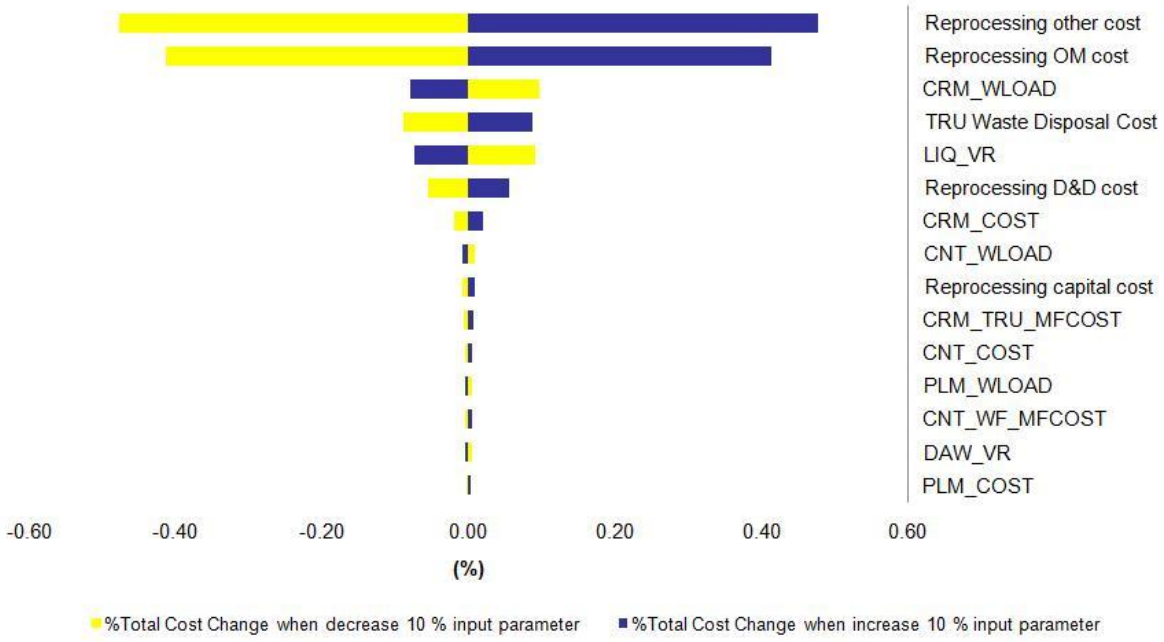


Figure 4-2 Sensitivity study chart on total cost

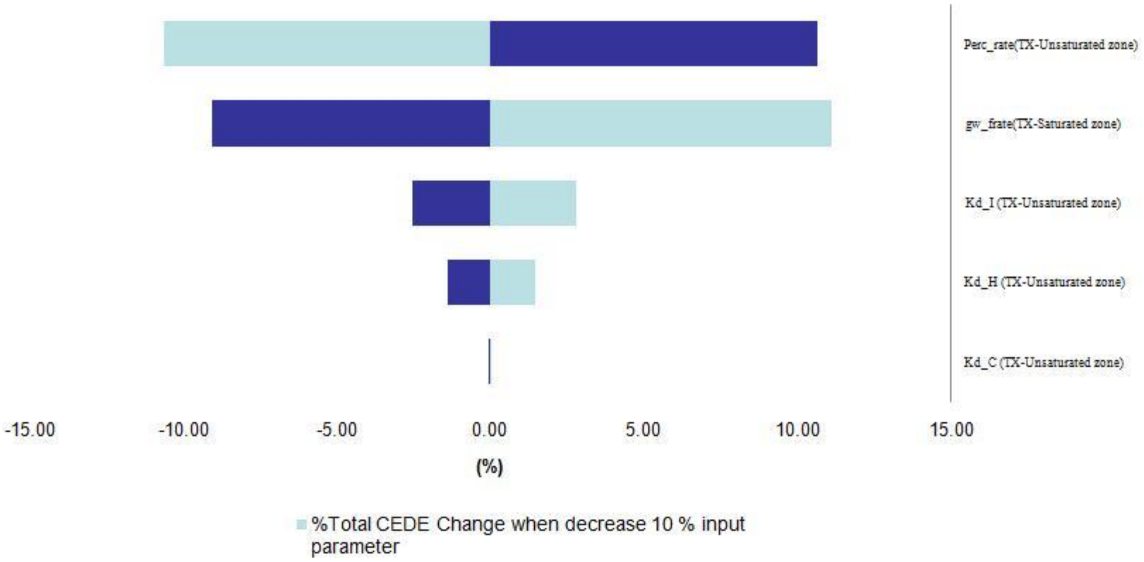


Figure 4-3 Sensitivity study chart on average CEDE

Table 4-1 and Table 4-2 show the 15 most sensitive input parameters to total cost and the 5 most sensitive input parameters to CEDE that were used in the probabilistic calculations, respectively. The true probability distributions of most of these parameters are usually not available; the most likely information that can be found is their ranges. For these cases, the distributions were assumed to be uniform within these ranges unless better representative distributions were defined. In the case when the probability distribution was not available and only a single value was obtained, the uniform distribution with the range extended (50% of both directions) from the single value was assumed. In the case that for some parameters, the distribution coefficient for certain elements was not available, those values were assumed to be the same as the data of the same group element.

Table 4-1 List of the input parameters that are most sensitive to total cost

Input parameter	Distribution	Low value	High value	Nominal	Reference
Reprocessing Capital Cost (USD/kg HM)	Triangle	268.83	397.96	315.00	[4]
Reprocessing O&M Cost (USD/kg HM)	Triangle	13270.22	19905.33	15672.50	[4]
Reprocessing D&D Cost (USD/kg HM)	Triangle	1788.70	2545.00	2117.67	[4]
Reprocessing Others Cost (USD/kg HM)	Triangle	15509.79	22757.72	18078.00	[4]
TRU Waste Disposal Cost (USD/L of final WF)	Uniform	511.55	517.12	517.12	[88]
Ceramic WF Manufacturing Cost for TRU Waste (USD/Liter of TRU waste stream)	Uniform	15.07	43.45	29.26	[89]
Ceramic Waste Loading (%)	Uniform	40.00	72.93	56.47	[90]
Ceramic Cost (USD/L of ceramic)	Uniform	60.00	180.00	120.00	[91][92]
Concrete WF Manufacturing Cost (USD/Liter of TRU waste stream)	Uniform	6.95	23.45	15.20	[91][92]
Concrete Waste Loading (%)	Uniform	10.00	50.00	30.00	[46]
Concrete Cost (USD/L of concrete)	Uniform	15.00	45.00	30.00	NA
Polymer Waste Loading (%)	Uniform	30.00	40.00	35.00	[46]
Polymer Cost (USD/L of polymer)	Uniform	30.00	90.00	60.00	NA

Table 4-1 Continued

Input parameter	Distribution	Low value	High value	Nominal	Reference
Dry Solid Waste Volume Reduction Ratio	Uniform	3.00	10.00	6.50	[46]
Liquid Waste Volume Reduction Ratio	Uniform	2.00	4.00	3.00	[46]

Note for ceramic waste form, cost data were assumed to be 20% greater than the cost for glass waste form.

Table 4-2 List of the input parameters that are most sensitive to CEDE

Input parameter	Distribution	Low value	High value	Nominal	Reference
Percolation rate ($\frac{m}{y}$) at Texas LLW site	Uniform	0.193	0.787	0.387	[gg]
Groundwater discharge ($\frac{m^3}{y}$) at Texas LLW site	Uniform	5186550	15560000	7056600	[93]
Sorption coefficient for Iodine ($\frac{mL}{g}$) for groundwater system at Texas LLW site	Uniform	0	0.20	0.10	[85]
Sorption coefficient for Hydrogen ($\frac{mL}{g}$) for groundwater system at Texas LLW site	Uniform	0	0.25	0.13	[85]
Sorption coefficient for Carbon ($\frac{mL}{g}$) for groundwater system at Texas LLW site	Uniform	0	0.25	0.13	[85]

A sensitivity study on expert weight was also performed. Because the decision weight could not be altered during the calculation because their summation must be equal to unity, the sensitivity methodology applied to regular input parameters was not applicable to the decision weights. The calculation was done by simply running the probabilistic calculations with different decision weights set at the very beginning of the simulation. The results for this study are shown in Table 4-3.

[gg] http://www.urs-slc.com/wcs/

Table 4-3 Sensitivity study results on various expert weights

Output	Value		
	Expert #1	Expert #2	Equal weights
Costs (million USD/MTHM)	237.30±1.32	237.40±1.56	238.09±1.47
Average CEDE (mrem/y)	2.60E-03±1.44E-03	2.51E-03±1.23E-03	2.48-03±1.158E-03
Maximum CEDE (mrem/y)	5.75E-02±3.35E-02	5.49E-02±2.80E-02	5.43E-02±2.69E-02
HLW (m^3/MTHM)	6.19E-04±2.25E-04	7.10E-04±4.21E-04	6.10E-4±2.15E-4
LLW (m^3/MTHM)	7.13±3.80	7.02±3.05	7.11±3.59
TRU Waste (m^3/MTHM)	4.41±1.09	4.42±1.15	6.59±1.50
MLLW (m^3/MTHM)	4.52±2.24	4.46±2.04	4.37±2.00

4.3 UREX case study results

In order to get probabilistic results, repeated calculations or iterations (using @Risk software) must be performed as explained in the introduction section in Chapter 3. Due to time constraints, only 100 iterations were performed in order to demonstrate the capability of the code. However, a more accurate probabilistic calculation could be performed, a greater number of iterations, if needed. The summary of the calculation results using the average of the expert decision weights are given in Table 4-4. Please see Appendix H for more detailed results.

Table 4-4 IWMS global outputs

Output	Mean	Standard deviation
Costs (million USD/MTHM)	237.39	1.42
Average CEDE (mrem/y)	2.61E-03	1.43E-03
Maximum CEDE (mrem/y)	5.78E-02	3.35E-02
HLW Volume (m^3/MTHM)	6.15E-04	2.19E-04
LLW Volume (m^3/MTHM)	7.03	3.98
TRU Waste Volume (m^3/MTHM)	4.43	1.25
MLLW Volume (m^3/MTHM)	4.52	2.40

Although different kinds of calculation results can be obtained from IWMS, only relevant ones are presented here. They are the waste streams from all associated processes along with their important properties, their best management alternatives and costs associated with the selected alternatives. Table 4-5 and 4-6 show summaries of these results.

Table 4-5 IWMS suggested management alternatives to direct waste streams associated with the UREX process

Stream description	Form	Classification	WM Alternative
DISBT2P1/Activated Metals	Metal	GTCCHW	DD_MET
DISST2P1/Non-Dissolved Solid	In	TRU	DD_CRM
DISST2P2/Empty Hull	Metal	TRU	DD_MET
UREXT2P1/Tc	In-H	C	DD_CNT
UREXT2P2/Wash effluent	In-H	A	EXEMPT
UREXT2P3/Spent solvent	Or-H	TRU	DD_CRM
UREXT1P2/Raffinate	In-H	TRU	DD_CRM
OFGTT2P1/C-14	In	C	DD_CNT
OFGTT2P2/H-3	Or	B	DD_PLM
OFGTT2P3/I-129	In	GTCCLW	DD_CNT
OFGTT2P4/Kr-85	In	B	DD_CNT

"In-H" denotes the unprocessed waste stream is in an inorganic form and contains chemically hazard material. "Or-H" denotes the unprocessed waste stream is in an organic form and contains a chemically hazardous material. "In" and "Or" denote the unprocessed wastes streams in an inorganic and an organic forms, respectively and does not contain chemically hazardous material. "DD_MET", "DD_CRM", "DD_CNT", "DD_PLM", "DD_GLS" denote waste management choice of direct disposal with waste form material of metal, ceramic, concrete, polymer and glass respectively.

Table 4-6 IWMS suggested management alternatives to secondary waste streams associated with the UREX process

Stream description	Form	Classification	WM Alternative
DISSLiq_Aq	In	A	DD_CNT
DISSResin	Or	A	DD_PLM
DISSFilter	Or	A	DD_PLM
DISSTech	In	A	DD_CNT
UREXLiq_Aq	In	TRU	DD_CRM
UREXLiq_Or	Or	TRU	DD_CRM
UREXFilter	Or	A	DD_PLM
UREXTech	In	A	DD_CNT
UREXEquip	In	A	DD_CNT

Table 4-6 Continued

Stream description	Form	Classification	WM Alternative
MOXFUELLiq_Aq	In	A	EXEMPT
MOXFUELLiq_Or	Or	A	EXEMPT
MOXFUELFilter	Or	A	EXEMPT
MOXFUELTech	In	A	EXEMPT
MOXFUELEquip	In	A	EXEMPT
OFGTLiq_Aq	In	A	DD_CNT
OFGTResin	Or	A	DD_PLM
OFGTFilter	Or	A	DD_PLM
OFGTEquip	In	A	DD_CNT
OFGTMixed	Mixed	A	DD_CNT

Some of the input parameters were unavailable so values were assumed; hence the calculation results presented are subjective and for demonstration purposes only. They should be referred to with careful consideration.

Based on Table 4-5 and Table 4-6, the majority of the best management alternatives were direct disposal with various types of waste form materials depending on the streams. Although some of the input parameters used were assumed, the overall results seem reasonable and agree with the current waste management policy, i.e. direct disposal. The only difference was whether they would be disposed of as LLW or HLW or others. The current regulations state that the waste from reprocessing must be treated as HLW hence it must be disposed of at the geologic repository. That means the wastes in Table 4-5 would be treated as HLW and eventually disposed of at the YMF. Managing wastes based on their inherent properties (not their origins) might help not only in replacing some of the HLW that must be stringently and expensively managed with LLW ones (easier and cheaper to manage) but also in improving the capacity issues of the YMF. Table 4-6 shows that most of the secondary waste streams be treated as LLW, with several streams being discarded.

4.4 Waste Management Scenario Applications

IWMS can also be used to compare user created waste management scenario. Although the only UREX process was the only process being compared to the actual experimental data, a relative comparison of UREX+ processes using the IWMS tool is valid. Four more UREX based process scenarios were analyzed with respect to the reference UREX process where all waste streams would be vitrified in borosilicate glass. The first scenario was UREX process with IWMS waste optimizations. The second scenario was UREX plus CCD/PEG with IWMS waste optimizations. The third scenario was UREX plus CCD/PEG with vitrification of all the waste streams. The forth scenario was UREX plus CCD/PEG with vitrification of all the waste streams but storage of Cs/Sr. The global outputs being compared are shown in Table 4-7.

Table 4-7 Comparison of waste management scenarios

Scenario #	Reprocessing Cost (USD/MTHM)	Waste Management Cost (USD/MTHM)	CEDE (mrem/y)	HLW and TRU (m^3/MTHM)	LLW (m^3/MTHM)
Reference	239±1.19		7.33E-07±3.73E-07	6.17±1.18	6.25±2.25
1	237±1.42		2.61E-03±1.43E-03	4.39±1.23	11.7±4.59
2	249±2.11		1.98E-03±8.89E-04	11.7±2.58	25.3±10.8
3	250±2.15		5.93E-07±3.54E-07	13.5±2.52	12.1±2.58
4	250±2.23		5.80E-07±3.22E-07	13.5±2.44	8.71±2.11

Chapter 5 Conclusions and Future Work

Integrated Waste Management Simulation (IWMS) code was developed by combining; (1) a simple reprocessing model to estimate the amount of by products derived from an advanced aqueous separation process, (2) a general waste management model to determine the attributes of waste streams, used in nuclear waste management alternatives pre-selection process, (3) a multiple criteria decision analysis model to suggest the preferred management alternative to the derived streams from the advanced separation process. The case study has demonstrated that simple and straight forward methodology in IWMS modeling could be used to determine the total cost of the UF reprocessing and the cost of the management by its products as well as identify key parameters that contribute the most effect to the total cost. The IWMS code could be also used to determine the volume of final waste forms and their preferred management strategies from a given reprocessing scheme such as UREX. The IWMS input parameters and their probabilistic distributions could be manipulated with ease via user-interface spreadsheet which allows the user to refine input parameters when needed and specifically investigate the problem at hand. Because of limited information availability (some data are classified and some do not exist), the closest possible comparison performed was the UREX process benchmarking (as explained in chapter 3). IWMS involves significant amounts of input parameters, some of which were subjective and some of which were assumed just to demonstrate the methodology and the model itself. Hence the result of the case study should be referred to with careful considerations.

Regardless of this limitation, IWMS could serve as a screening tool to investigate the relative questions such as how much waste would be produced from UREX versus UREX+1, and what would be the best waste management option for their by products (once the more detailed data for the FPEX, TRUEX and TALSPEAK separation processes become available).

Most of the models used in IWMS are simple, especially the solvent extraction models that employed equilibrium conditions which may lack of the capability to capture the kinetics of the reactions that influence the final volume of the process streams, i.e. raw material streams, product streams. The future work regarding the solvent extraction model that needs to be done is:

- The current solvent extraction model does not take into account the fact that the costs of separation are affected by target separation efficiencies, i.e. 99% or 99.99 % U recovery will change the cost of U extraction. The more refined liquid-liquid extraction model that can determine the number of extraction stage should be employed in order to capture better cost estimates for the process.
- Because the radioactivity of the contaminated wastes is a key to determine the classification of such stream in the IWMS modeling and in order to model the radioactivity contained in certain streams, more detailed information on the contamination factors (α) during the reprocessing process should be accurately defined, whether or not this parameter is affected by the radioactivity level of the incoming UF.

Since most of the information used in the IWMS modeling is hard to find or unavailable and was assumed in the calculation, gathering the more detailed data is an essential on-going task. The input parameters that need to be updated can be listed as follows:

- Steady state volumetric flow parameters for all the advanced aqueous separation processes (except UREX) and their associated secondary wastes as well as their costs (i.e. process capital cost; operation and maintenance costs; decontamination and disposal costs; and raw material costs).
- The cost information for ceramic and polymer waste forms manufacturing as well as more refined cost information for glass, metal and concrete waste forms manufacturing.
- The cost data for the decontamination of all radionuclides that are assumed recyclable and their market values.
- The waste information for the transmutation option and the cost that is associated with it.
- Sorption or distribution coefficient of most elements for groundwater transport calculation in the specified system, i.e. the YMF and LLW disposal site, Andrews County, TX.

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Appendix

Appendix A List of streams for advanced aqueous separation processes

Process	Stream #	Stream Type	Stream Code	Stream Description
DISB	1	Type II Input #1	DISBT2RM1	Spent fuel assemblies
	2	Type I Output #1	DISBT1P1	Spent fuel rods
		Type I Output #2	DISBT1P2	Structured materials
CHOP	1	Type I Input # 1	CHOPT1RM1	Spent fuel rods
	2	Type I Output # 1	CHOPT1P1	Chopped fuel rods
		Type I Output # 2	CHOPT1P2	Off-gas (1)
	1	Type II Output # 1	CHOPT2P1	Scrap metal
VOLX	1	Type I Input # 1	VOLXT1RM1	Chopped fuel rods
	2	Type I Output # 1	VOLXT1P1	Fuel powder
		Type I Output # 2	VOLXT1P2	Off-gas
	1	Type II Output # 1	VOLXT2P1	Empty hulls
DISSV	1	Type I Input # 1	DISST1RM1	Fuel powder
	1	Type II Input # 1	DISST2RM1	Nitric acid
	1	Type I Output #1	DISST1P1	Fuel solution
DISSC	1	Type I Input # 1	DISST1RM1	Chopped fuel rods
	1	Type II Input # 1	DISST2RM1	Nitric acid
	2	Type I Output #1	DISST1P1	Fuel solution
		Type I Output #2	DISST1P2	Off-gas
	2	Type II Output #1	DISST2P1	Non dissolved solids
		Type II Output #2	DISST2P2	Empty hulls
UREX	1	Type I Input # 1	UREXT1RM1	Spent fuel solution
	7	Type II Input # 1	UREXT2RM1	Tri Butyl Phosphate (TBP)
		Type II Input # 2	UREXT2RM1	Dodecane
		Type II Input # 3	UREXT2RM1	0.3 M Nitric acid (Scrub)
		Type II Input # 4	UREXT2RM1	0.01 M Nitric acid (U strip)
		Type II Input # 5	UREXT2RM1	6.0 M Nitric acid (Tc strip)
		Type II Input # 6	UREXT2RM1	Dilute Nitric acid (Wash)
		Type II Input # 7	UREXT2RM1	Acetohydroxamic acid (AHA)
	2	Type I Output #1	UREXT1P1	U Product
		Type I Output #2	UREXT1P2	UREX raffinate
	3	Type II Output #1	UREXT2P1	Tc Product
		Type II Output #2	UREXT2P2	Wash effluent
		Type II Output #3	UREXT2P3	Spent solvent
COEX	1	Type I Input # 1	COEXT1RM1	Spent fuel solution
	11	Type II Input # 1	COEXT2RM1	Tri Butyl Phosphate (TBP)
		Type II Input # 2	COEXT2RM2	Dodecane
		Type II Input # 3	COEXT2RM3	Concentrated Nitric acid (FP Scrub)
		Type II Input # 4	COEXT2RM4	Dilute Nitric acid (Zr Scrub)
		Type II Input # 5	COEXT2RM5	Nitric acid (Pu/Np Scrub)
		Type II Input # 6	COEXT2RM6	Complexant (Pu/Np Strip)
		Type II Input # 7	COEXT2RM7	Dilute Nitric acid (Pu/Np Strip)
		Type II Input # 8	COEXT2RM8	Nitric acid (AHA Scrub)
		Type II Input # 9	COEXT2RM9	Nitric acid (U/Tc Strip)
		Type II Input # 10	COEXT2RM10	Nitric acid (Wash)
		Type II Input # 11	COEXT2RM11	Elute solution
	2	Type I Output #1	COEXT1P1	U product
		Type I Output #2	COEXT1P2	COEX raffinate
	4	Type II Output #1	COEXT2P1	Tc
		Type II Output #2	COEXT2P2	Pu/Np
		Type II Output #3	COEXT2P3	Wash effluent
		Type II Output #4	COEXT2P4	Spent solvent

Process	Stream #	Stream Type	Stream Code	Stream Description
FPEX	1	Type I Input # 1	FPEXT1RM1	UREX/COEX raffinate
	8	Type II Input # 1	FPEXT2RM1	DtBuCH18C6a
		Type II Input # 2	FPEXT2RM2	BOBCalixb
		Type II Input # 3	FPEXT2RM3	Trioctylamine (TOA)
		Type II Input # 4	FPEXT2RM4	Cs-7SB cmodifier
		Type II Input # 5	FPEXT2RM5	Isopar L diluent
		Type II Input # 6	FPEXT2RM6	Nitric acid (Scrub)
		Type II Input # 7	FPEXT2RM7	Nitric acid (Strip)
		Type II Input # 8	FPEXT2RM8	Nitric acid (Wash)
	1	Type I Output #1	FPEXT1P1	FPEX raffinate
	3	Type II Output #1	FPEXT2P1	Cs/Sr/Ba/Rb
		Type II Output #2	FPEXT2P2	Wash effluent
		Type II Output #3	FPEXT2P3	Spent solvent
CCDPEG	1	Type I Input # 1	CCDPEGT1RM1	UREX/COEX raffinate
	8	Type II Input # 1	CCDPEGT2RM1	CCDd
		Type II Input # 2	CCDPEGT2RM2	Poly Ethylene glycol (PEG)
		Type II Input # 3	CCDPEGT2RM3	FS-13e
		Type II Input # 4	CCDPEGT2RM4	DTPAf
		Type II Input # 5	CCDPEGT2RM5	Guanidine Carbonate
		Type II Input # 6	CCDPEGT2RM6	Nitric acid (Scrub)
		Type II Input # 7	CCDPEGT2RM7	PEG (Wash)
		Type II Input # 8	CCDPEGT2RM8	Nitric acid (Wash)
	1	Type I Output #1	CCDPEGT1P1	CCDPEG raffinate
	3	Type II Output #1	CCDPEGT2P1	Cs/Sr/Ba/Rb
		Type II Output #2	CCDPEGT2P2	Wash effluent
		Type II Output #3	CCDPEGT2P3	Spent solvent
TRUEX	1	Type I Input # 1	TRUEXT1RM1	FPEX/CCDPEG raffinate
	11	Type II Input # 1	TRUEXT2RM1	CMPOg
		Type II Input # 2	TRUEXT2RM2	Tri Butyl Phosphate (TBP)
		Type II Input # 3	TRUEXT2RM3	Dodecane
		Type II Input # 4	TRUEXT2RM4	Complexant
		Type II Input # 5	TRUEXT2RM5	Diluted HNO3
		Type II Input # 6	TRUEXT2RM6	Conc HNO3 (Scrub1)
		Type II Input # 7	TRUEXT2RM7	Dilute HNO3 (Scrub2)
		Type II Input # 8	TRUEXT2RM8	Lactic acid (Strip)
		Type II Input # 9	TRUEXT2RM9	DTPA (Strip)
		Type II Input # 10	TRUEXT2RM10	Wash solution
		Type II Input # 11	TRUEXT2RM11	Feed adjust reagent
	1	Type I Output #1	TRUEXT1P1	TRU/LN
	4	Type II Output #1	TRUEXT2P1	TRUEX raffinate (Major remaining FPs)
		Type II Output #2	TRUEXT2P2	Wash effluent
		Type II Output #3	TRUEXT2P3	Feed adjusted effluent
		Type II Output #4	TRUEXT2P4	Spent solvent

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[a] 4,4',(5')-Di-(t-butyldicyclo-hexano)-18-crown-6 :DtBuCH18C6

[b] Calix[4]arene-bis-(tertoctylbenzo-crown-6) : BOBCalix

[c] 1-(2,2,3,3-tetrafluoropropoxy)-3-(4-sec-butylphenoxy)-2-propanol: Cs-7SB

[d] Chlorinated Cobalt Dicarbollide (CCD)

[e] Phenyltrifluoromethyl Sulfone (FS-13)

[f] Diethylene triamine pentaacetic acid (DTPA)

[g] Octyl(Phenyl)-N,N-diisobutylcarbamoyl methyphosphine oxide (CMPO)

Process	**Stream #**	**Stream Type**	**Stream Code**	**Stream Description**
TALSPEAK	1	Type I Input # 1	TALSPEAKT1RM1	TRUEX Loaded solvent
	8	Type II Input # 1	TALSPEAKT2RM1	HDEHPh
		Type II Input # 2	TALSPEAKT2RM2	Dodecane
		Type II Input # 3	TALSPEAKT2RM3	Lactic acid
		Type II Input # 4	TALSPEAKT2RM4	DTPA
		Type II Input # 5	TALSPEAKT2RM5	Conc HNO3
		Type II Input # 6	TALSPEAKT2RM6	Wash solution
		Type II Input # 7	TALSPEAKT2RM7	Feed adjust Lactic acid
		Type II Input # 8	TALSPEAKT2RM8	Feed adjust DTPA
	1	Type I Output #1	TALSPEAKT1P1	TRU (TALSPEAK Raffinate)
	4	Type II Output #1	TALSPEAKT2P1	Lanthanides (Stripped)
		Type II Output #2	TALSPEAKT2P2	Wash effluent
		Type II Output #3	TALSPEAKT2P3	Feed adjusted effluent
		Type II Output #4	TALSPEAKT2P4	Spent solvent
REVTAL	1	Type I Input # 1	REVTALT1RM1	TRUEX Loaded solvent
	7	Type II Input # 1	REVTALT2RM1	HDEHP
		Type II Input # 2	REVTALT2RM2	Dodecane
		Type II Input # 3	REVTALT2RM3	Conc HNO3 (Zr scrub)
		Type II Input # 4	REVTALT2RM4	DTPA
		Type II Input # 5	REVTALT2RM5	Lactic acid
		Type II Input # 6	REVTALT2RM6	Dilute HNO3 (Ln strip)
		Type II Input # 7	REVTALT2RM7	Wash solution
	1	Type I Output #1	REVTALT1P1	TRU Product(Stripped)
	4	Type II Output #1	REVTALT2P1	Lanthanides(Stripped)
		Type II Output #2	REVTALT2P2	REVTAL raffinate
		Type II Output #3	REVTALT2P3	Wash effluent
		Type II Output #3	REVTALT2P4	Spent solvent
MOXFUEL	1	Type I Input # 1	MOXFUELT1RM1	U products
	2	Type II Input # 1	MOXFUELT2RM1	PuO2
		Type II Input # 2	MOXFUELT2RM2	Additives
	2	Type II Output #1	MOXFUELT2P1	MOX fuel
		Type II Output #2	MOXFUELT2P2	Nitric acid
NEXFUEL	1	Type I Input # 1	NEXFUELT1RM1	TRU products
	2	Type II Input # 1	NEXFUELT2RM1	Y Zr Nitrate solution
		Type II Input # 2	NEXFUELT2RM2	Metal powder
	1	Type II Output #1	NEXFUELT2P1	Next generation fuel

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[h] Di-(2-ethylhexyl) phosphoric acid (HDEHP)

Process	**Stream #**	**Stream Type**	**Stream Code**	**Stream Description**
OFGTV	2	Type I Input # 1	OFGTT1RM1	Off-gas
		Type I Input # 2	OFGTT1RM2	Off-gas
	6	Type II Input # 1	OFGTT2RM1	Raw material #1
		Type II Input # 2	OFGTT2RM2	Raw material #2
		Type II Input # 3	OFGTT2RM3	Raw material #3
		Type II Input # 4	OFGTT2RM4	Raw material #4
		Type II Input # 5	OFGTT2RM5	Raw material #5
		Type II Input # 6	OFGTT2RM6	Raw material #6
		Type II Input # 7	OFGTT2RM7	Raw material #7
	6	Type II Output #1	OFGTT2P1	C-14
		Type II Output #2	OFGTT2P2	H-3
		Type II Output #3	OFGTT2P3	I-129
		Type II Output #4	OFGTT2P4	Kr-85
		Type II Output #5	OFGTT2P5	Cs
		Type II Output #6	OFGTT2P6	Tc
		Type II Output #7	OFGTT2P7	Ru
OFGTC	2	Type I Input # 1	OFGTT1RM1	Off-gas
		Type I Input # 2	OFGTT1RM2	Off-gas
	2	Type II Input # 1	OFGTT2RM1	Raw material #1
		Type II Input # 2	OFGTT2RM2	Raw material #2
		Type II Input # 3	OFGTT2RM3	Raw material #3
		Type II Input # 4	OFGTT2RM4	Raw material #4
	4	Type II Output #1	OFGTT2P1	C-14
		Type II Output #2	OFGTT2P2	H-3
		Type II Output #3	OFGTT2P3	I-129
		Type II Output #4	OFGTT2P4	Kr-85

Appendix B Secondary waste code and descriptions

Table B-1 Secondary wastes from any process in general

Code	**Material type**
XXXXmetal	Contaminated Metal from given process
XXXXLiq_Aq	Aqueous liquid
XXXXLiq_Or	Organic liquid
XXXXSludge	Sludge
XXXXResin	Spent resin
XXXXFilter	Used filter
XXXXTech	Technological waste
XXXXEquip	Contaminated equipment
XXXXAsh	Ash
XXXXMixed	Mixed waste
XXXXMisc1	Miscellaneous1
XXXXMisc2	Miscellaneous 2

Table B-2 Secondary wastes from UREX process

Code	**Material type**
UREX metal	Contaminated Metal from given process
UREXLiq_Aq	Aqueous liquid
UREXLiq_Or	Organic liquid
UREXSludge	Sludge
UREXResin	Spent resin
UREXFilter	Used filter
UREXTech	Technological waste
UREXEquip	Contaminated equipment
UREXAsh	Ash
UREXMixed	Mixed waste
UREXMisc1	Miscellaneous1
UREXMisc2	Miscellaneous 2

Appendix C Flow diagram and assumptions of IWMS processes

Disassembling process

Process assumptions:

(a) There is no fuel rupture, i.e. fission product migration beyond cladding material is negligible. Hence secondary waste derived from disassembling process is also negligible.

(b) Only activation products presented in cladding and structured materials.

(c) Simple mass balance calculation model.

Process descriptions:

(a) One input stream of type II—UF fuel assembly with maximum number of existing radionuclide in the stream equal nuc_count. This stream is supplied by AFC model.

(b) Two supports inputs under the same stream—Activation products inventories in cladding material and structured materials. Maximum number of radionuclides presented in cladding and structured materials are nclad and nss respectively.

(c) Two output streams of type I—used fuel rods and structured material with maximum number of existing radionuclide in the stream equal nuc_count+nclad and nss respectively.

Mass balance:

(a) Isotropic concentration of activation products of cladding and structured materials were estimated using ORIGEN ARP.

(b) The isotropic concentration of activation products was normalized to 1 Metric ton Uranium (MTU) of PWR fuel. The following parameters were used in the model for normalization purposes;

- Volume of fuel meat (UO2) of 9.1924D1 liters of UO2 per MTU
- Volume of fuel clad of 1.31578D2 liters per MTU was estimated using Turkey Point Unit 3 PWR assembly description
- Volume of structured materials (stainless steel) of 1.31578D2 liters per MTU was assumed. More accurate number is needed.
- Density of fuel meat of 1.097D1 kg per liter of UO2[i]
- Density of fuel clad of 6.44D0 kg per liter[j]
- Density of structure materials of 7.9D0kg per liter [k]

(C) Volume of fuel rod (DISBT1P1) was calculated as followed;

Volume of fuel rod = Volume of fuel meat + Volume of fuel clad

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[i] http://en.wikipedia.org/wiki/Uranium_dioxide
[j] http://www.engr.utk.edu/org/ans/benchmark/ansmox_2bench.html
[k] http://wiki.answers.com/Q/What_is_density_of_304_grade_stainless_steel

Chopping process

Process assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed.

(b) Scrap production fraction (F_SCP) is uniform for all fission and activation elements, after fission gas has been released from the fuel.

(c) Fission gas release fraction (Xx_Frac_CH) is constant for all gaseous isotopes of the same volatile element. Different elements have different release fraction which are supplied through "HeadendParameters" spreadsheet.

(d) Number of fission gas is fixed at 4 radionuclides (C-14, H-3, I-129, Kr-85).

(e) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

(f) Constant volume of FP volatile material (FP_vol_V) of 878.0398 L/MTU, was assumed based on 27620 MWD/MTU burnup[]. The fraction of FP gas assumed release during chopping process is 0.3. The rest is assumed to release either during voloxidation or dissolution process

Process descriptions:

(a) One input stream of type I—SNF fuel rods with maximum number of existing radionuclide in the stream equal nuc_count+nclad. This stream is calculated internally in IWMS model via "DISB_BOX" subroutine.

(b) Two output streams of type I —fuel hulls and fission gas with maximum number of existing radionuclide in the stream equal nuc_count+nclad and 4 respectively. These two streams are determined via "CHOP_BOX" subroutine.

(c) One output stream of type II—scrap metals with maximum number of existing radionuclide in the stream equal nuc_count+nclad. This stream is also determined via "CHOP_BOX" subroutine.

Mass balance:

Figure 3-3 illustrates how mass balances of radionuclides distributed throughout voloxidation process are determined.

Voloxidation process

Process assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed

(b) Fission gas release fraction (Xx_Frac_VX) is constant for all gaseous isotopes of the same volatile element. Different elements have different release fraction which are supplied through "HeadendParameters" spreadsheet. All volatile gas(C-14, H-3, I-129, Kr-85) have released fraction of 1.0 while semi-volatile material (all Cs and Tc isotopes) has released fraction of less than 1.0

(c) Total number of volatile and semi-volatile fission gas released during Voloxidation is fixed at nvolg (C-14, H-3, I-129, Kr-85, all Cs and Tc isotopes).

(d) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

(e) Constant volume of FP volatile material (FP_vol_V) of 878.0398 L/MTU, was assumed based on 27620 MWD/MTU burnup. The fraction of FP gas assumed release during chopping process is 0.5. The rest is assumed to release either during voloxidation or dissolution process.

(f) Constant volume of FP semi-volatile material (FP_vol_S) of 50.0 L/MTU, was assumed.

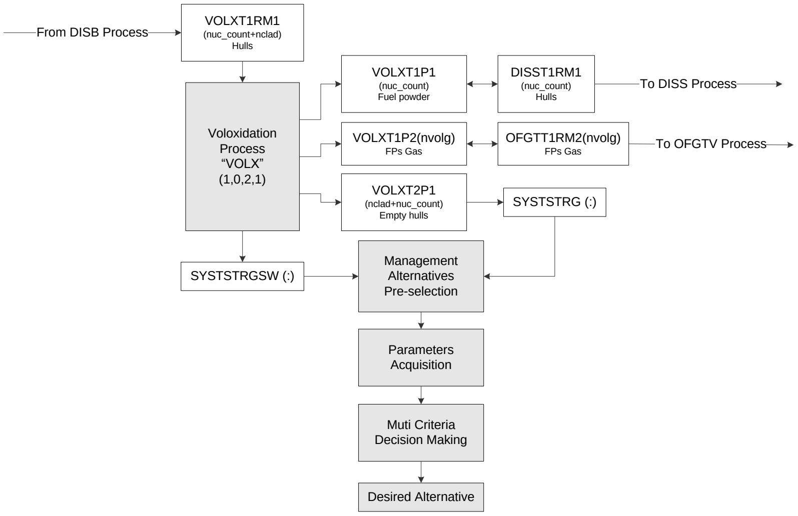

Figure C-1 Voloxidation process flow diagram

Process descriptions:

(a) One input stream of type I—Chopped fuel rods with maximum number of existing radionuclide in the stream equal nuc_count+nclad. This stream is calculated internally in IWMS model via "CHOP_BOX" subroutine.

(b) Two output streams of type I —fuel powder and fission gas with maximum number of existing radionuclide in the stream equal nuc_count and 4 respectively. These two streams are determined via "VOLX_BOX" subroutine.

(c) One output stream of type II—empty hulls with maximum number of existing radionuclide in the stream equal nuc_count+nclad. This stream is also determined via "VOLX_BOX" subroutine.

Mass balance:

Figure C-1 illustrates how mass balances of radionuclides distributed throughout voloxidation process are determined.

Dissolution process

Process assumptions:

(a) The Major calculation regarding dissolution process was included in subroutines "DISSC_BOX" and "DISSV_BOX" inherited in module name "BOXROUTINES".

(b) Required input information includes

(1) Necessary process parameters are included in the input file name "diss1_box.inp", "diss2_box.inp", and "diss3_box.inp" that are created by macro function in Excel spreadsheet and then imported into subroutines when needed.

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "dissc_sw.inp" and "dissv_sw.inp" that are created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed.

(b) Fission gas release fraction (Xx_Frac_DS) is constant for all gaseous isotopes of the same volatile element. Different elements have different release fraction which are supplied through "HeadendParameters" spreadsheet. All volatile gas(C-14, H-3, I-129, Kr-85) have released fraction of 1.0 while semi-volatile material (all Cs and Tc isotopes) is not released during dissolution process.

(c) Number of fission gas is fixed at 4 radionuclides (C-14, H-3, I-129, Kr-85).

(d) Constant volume of FP volatile material (FP_vol_V) of 1.96 L/MTU, was assumed based on 61.72 MWD/MTU burnup. The fraction of FP gas assumed release during chopping process is 0.3. The rest is assumed to release either during voloxidation or dissolution process.

(e) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

(f) Fraction for non-dissolved solid is 0.0 when voloxidation process is employed and equal to Xx_ndiseff_DS when voloxidation is not employed.

(g) Fraction for fission products in clad materials (Xx_clad_DS) are obtained from "HeadendParameters" spreadsheet as well as dissolution efficiencies (xx_diseff_DS).

(h) Uranium concentration in feed solution (Feed_conc) was assumed constant at 3.77E-2 g/L []. Total volume of nitric acid raw material is calculated based on uranium content in a given stream and this concentration.

(i) Concentrated nitric acid http://www.saichemicals.co.in/Nitric_acid.html

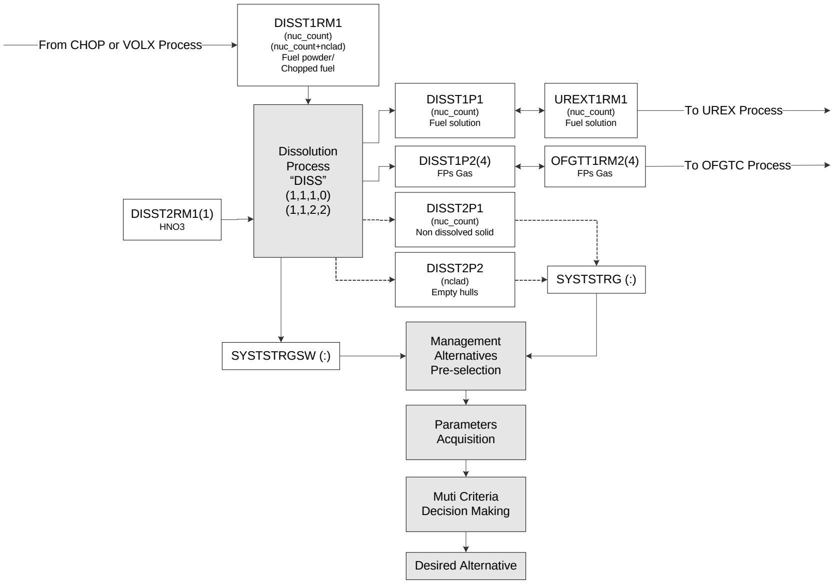

Figure C-2 Dissolution process flow diagram

Process descriptions:

(For DISSC)

(a) One input stream of type I—chopped fuel rods with number of existing radionuclide in the stream equal nuc_count+nclad. This stream is calculated internally in IWMS model via “CHOP_BOX” subroutine.

(b) One input stream of type II (raw material)—Nitric acid with no radioactive material presented in it.

(c) Two output streams of type I —used fuel solution and fission gas with number of existing radionuclide in the stream equal nuc_count and 4 respectively. These two streams are determined via “DISSC_BOX” subroutine.

(d) Two output streams of type II—empty hulls and non-dissolved solid with both number of existing radionuclide in the streams equal nuc_count+nclad. This stream is also determined via “DISSC_BOX” subroutine.

(For DISSV)

(a) One input stream of type I—fuel powder with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via “VOLX_BOX” subroutine.

(b) One input stream of type II (raw material)—Nitric acid with no radioactive material presented in it.

(c) One output stream of type I —used fuel solution with maximum number of existing radionuclides in the stream equal nuc_count. Since all fission gas was assumed released earlier during voloxidation. This stream is determined via “DISSV_BOX” subroutine.

(d) No output stream of type II—empty hulls are obtained earlier during voloxidation and non-dissolved solid is negligible since fuel powder can be dissolved effectively in nitric acid.

Mass balance:

Figure C-2 illustrates how mass balances of radionuclides distributed throughout dissolution process (when voloxidation is and is not considered) are determined.

UREX process

Process assumptions:

(a) The Major calculation regarding UREX process was included in subroutines “UREX_BOX” inherited in module name “BOXROUTINES”.

(b) Required input information includes

    (1) Input file name "urex_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed. Example of information in this input file are as followed; Steady state volumetric flow rate of each individual stream (input and output) of UREX process, needed for an estimation of reagents consumed in the process, was obtained from [WSRC-TR-2002-00444]. Mass fraction of U and Tc distributed in wash effluent was obtained from the same document (if applicable otherwise they are assumed).

    (2) Other process parameters specified inside the procedure themselves.

    (3) Radioactive waste associated with the process, which is included in the input file name "urex_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name "urex_cost.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

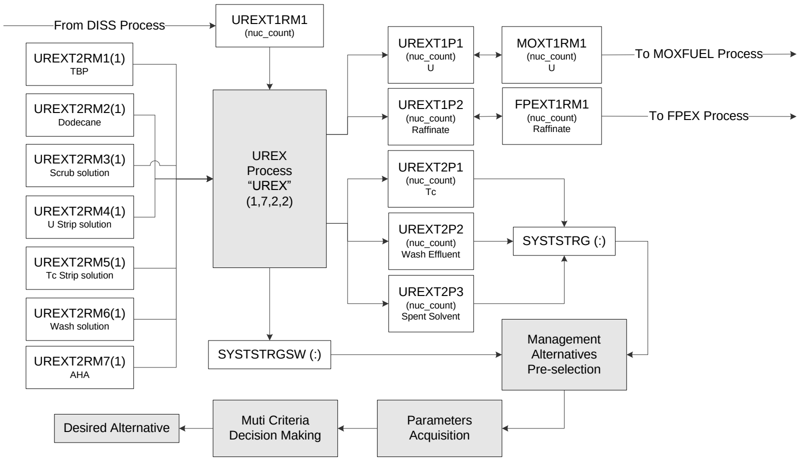

Figure C-3a UREX process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed based on the following stoichiometry.

H+(aq) + NO3-(aq) + TBP(or) <---> HNO3.TBP

UO2 2+(aq) + 2NO3-(aq) + 2TBP(or) <---> UO2(NO3)2.2TBP

H+(aq) + TcO4-(aq) + 2TBP(or) <---> HTcO4.2TBP

Mole TBP = 2*Mole initial U + 2*Mole initial Tc + Mole initial H

30% TBP in Dodecane by weight

Initial acid concentration is 1.0 M for UREX

(b) Steady state calculation with no loss due to third phase formation.

(c) Difference in 1st and 2nd cycles UREX is not taken into consideration. In this research, simplified UREX process box combines two UREX cycles and UREX solvent regeneration within it. Only relevant target efficiencies (one for U and one for Tc) are accounted for in UREX process.

(d) Since target separation efficiencies of the reprocessing for all key elements are set as individual single values which supplied by the AFC model.

(e) U and Tc are the only two elements that can be extracted into organic phase, hence no other nuclides presented in loaded solvent.

(f) Only interested product element is existed in its destination, i.e. there is solely U in U stripped product and only Tc in Tc-stripped product.

(g) Calculation of volume of raw material was based on steady state process proportionality flow rate. By assume that aqueous feed always has uranium content of 377 gram in 1 Liter of aqueous feed.

(h) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

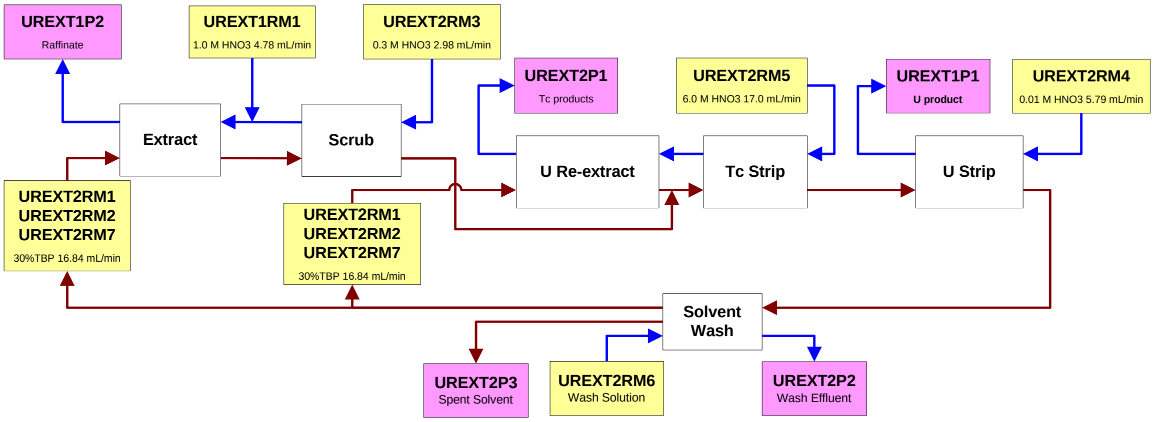

Figure C-3b UREX process streams flow

Process descriptions:

(a) One input stream of type I—used fuel solution with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via “DISSC_BOX” or “DISSV_BOX” subroutine.

(b) Seven input streams of type II (raw material)

(c) Two output streams of type I —U product and UREX raffinate with maximum number of existing radionuclide in both streams equal nuc_count. These two streams are determined via “UREX_BOX” subroutine.

(d) Two output streams of type II—Tc product and solvent wash effluent with maximum number of existing radionuclide in both streams equal nuc_count. This stream is also determined via “UREX_BOX” subroutine.

Mass balance:

Figure C-3a illustrates how mass balances of radionuclides distributed throughout UREX process

COEX process

Process assumptions:

(a) The Major calculation regarding COEX process was included in subroutines “COEX_BOX” inherited in module name “BOXROUTINES”.

(b) Required input information includes:

(1) Input file name "coex_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed. Example of information in this input file are as followed; Steady state volumetric flow rate of each individual stream (input and output) of COEX process, needed for an estimation of reagents consumed in the process, was obtained from []. Mass fraction of U, Tc, Pu and Np distributed in wash effluent was obtained from the same document (if applicable otherwise they are assumed).

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "coex_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name “coex_cost.inp” that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

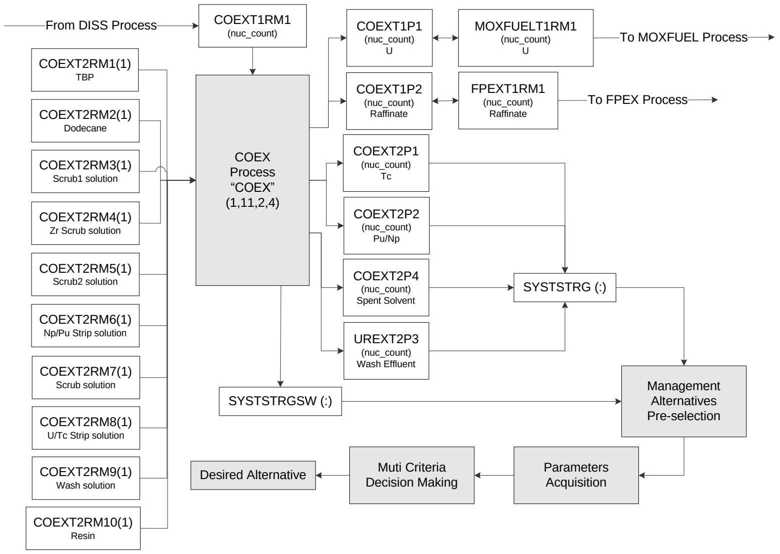

Figure C-4a COEX process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed

(b) Steady state calculation with no loss due to third phase formation.

(c) Target separation efficiencies of all key elements are supplied by the AFC model.

(d) U, Tc, Pu and Np are the only four elements that can be extracted into organic phase, hence no other nuclides presented in loaded solvent.

(e) Only interested product element is existed in its destination, i.e. there is solely U in U-stripped product, only Tc in Tc-stripped product and Pu/Np both in Pu/Np stripped product.

(f) Calculation of volume of raw material was based on steady state process proportionality flow rate. By assume that aqueous feed always has uranium content of 377 gram in 1 Liter of aqueous feed.

(g) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

(h) Tc is removed from U/Tc stripped product by anion exchanged process using Nitrated Reillex HPQ resin [94].

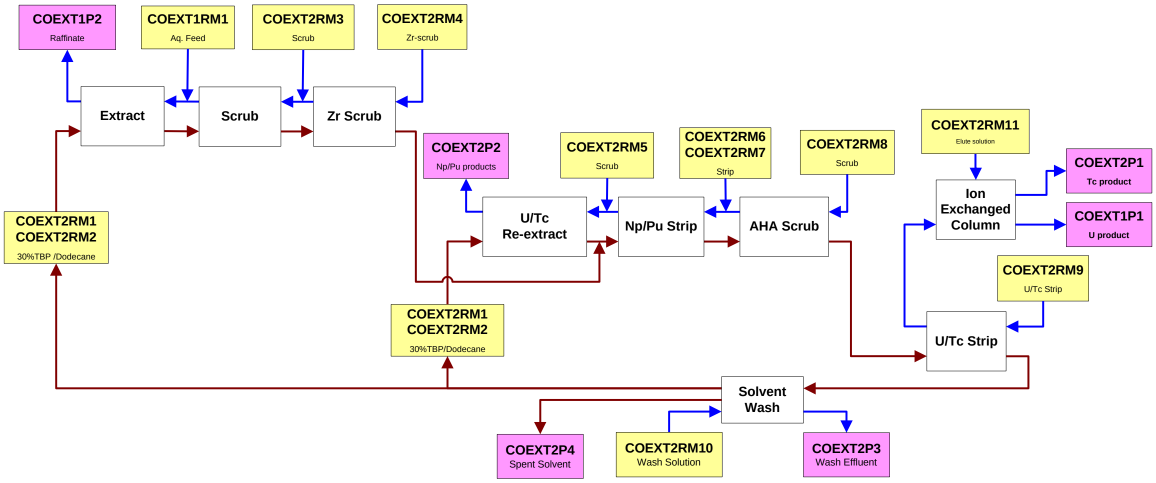

Figure C-4b COEX process streams flow

Process descriptions:

(a) One input stream of type I—used fuel solution with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via “DISSC_BOX” or “DISSV_BOX” subroutine.

(b) Eleven input streams of type II (raw material), all of them are chemical reagent used in COEX process.

(c) Two output streams of type I —U product and COEX raffinate with maximum number of existing radionuclide in the stream equal nuc_count. These two streams are determined via “COEX_BOX” subroutine.

(d) Four output streams of type II—Tc product, Pu/Np product and solvent wash effluent with maximum number of existing radionuclide in all streams equal nuc_count. This stream is also determined via “COEX_BOX” subroutine.

Mass balance:

Figure C4-a illustrates how mass balances of radionuclides distributed throughout COEX process.

FPEX Process

Process assumptions:

(a) The Major calculation regarding FPEX process was included in subroutines “FPEX_BOX” inherited in module name “BOXROUTINES”.

(b) Required input information includes:

(1) Input file name "fpex_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed. Example of information in this input file are as followed; Steady state volumetric flow rate of each individual stream (input and output) of FPEX process, needed for an estimation of reagents consumed in the process, was obtained from [21 ,95]. Mass fraction of Cs, Sr, Rb and Ba distributed in wash effluent was obtained from the same document (if applicable otherwise they are assumed).

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "fpex_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name “fpex_cost.inp” that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

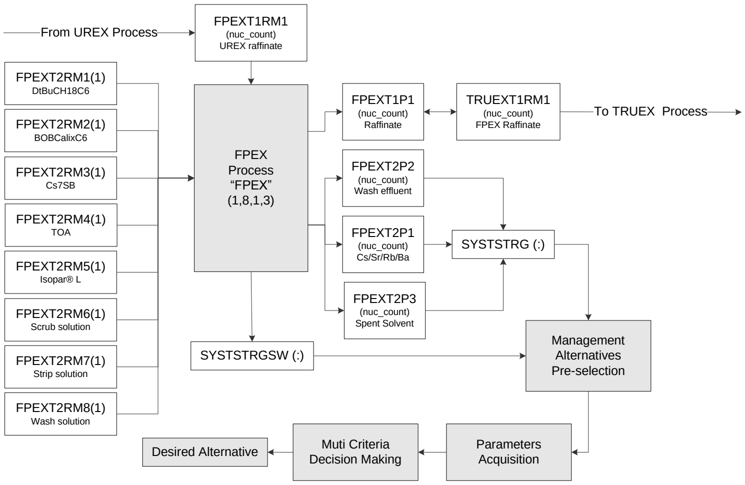

Figure C-5a FPEX process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed

(b) Steady state calculation with no loss due to third phase formation.

(c) Target separation efficiencies of all key elements are supplied by the AFC model.

(d) Cs, Sr Rb and Ba are the only four elements that can be extracted into organic phase, hence no other nuclides presented in loaded solvent.

(e) Only one interested product stream which contains Cs, Sr, Rb and Ba in stripped product. Other elements remain in raffinate.

(f) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

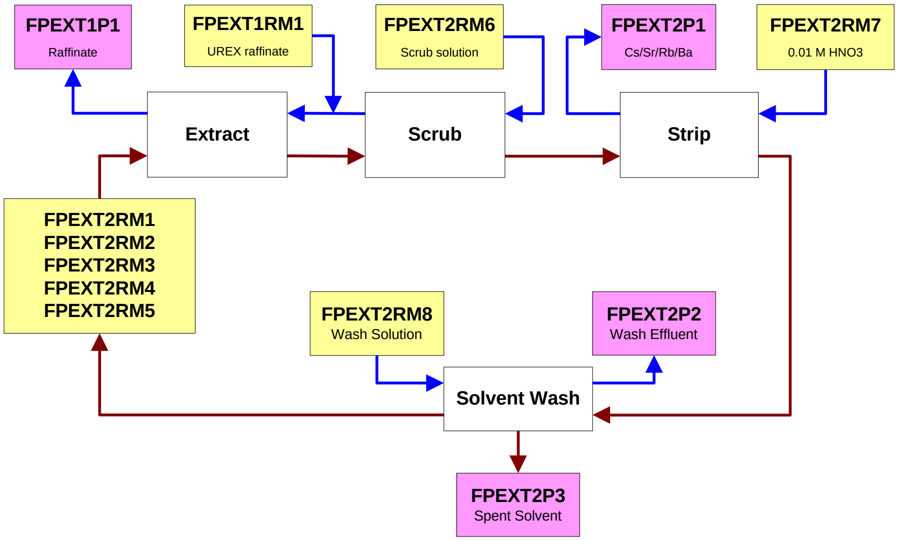

Figure C-5b FPEX process streams flow

Process descriptions:

(a) One input stream of type I—raffinate from UREX process with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via “UREX_BOX” subroutine.

(b) Eight input streams of type II (raw material), all of them are chemical reagent used in FPEX process.

(c) One output stream of type I —FPEX raffinate with maximum number of existing radionuclide in the stream equal nuc_count. This stream is determined via “FPEX_BOX” subroutine.

(d) Three output streams of type II— Cs/Sr.Rb/Ba product and solvent wash effluent with maximum number of existing radionuclide in all streams equal nuc_count. This stream is also determined via “FPEX_BOX” subroutine.

Mass balance:

Figure C5a illustrates how mass balances of radionuclides distributed throughout FPEX process.

CCDPEG process

Process assumptions:

(a) The Major calculation regarding CCDPEG process was included in subroutines “CCDPEG_BOX” inherited in module name “BOXROUTINES”.

(b) Required input information includes

(1) Input file name "ccdpeg_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed. Example of information in this input file are as followed; Steady state volumetric flow rate of each individual stream (input and output) of CCDPEG process, needed for an estimation of reagents consumed in the process, was obtained from [21 ,95] . Mass fraction of Cs, Sr, Rb and Ba distributed in wash effluent was obtained from the same document (if applicable otherwise they are assumed).

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "ccdpeg_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name “ccdpeg_cost.inp” that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

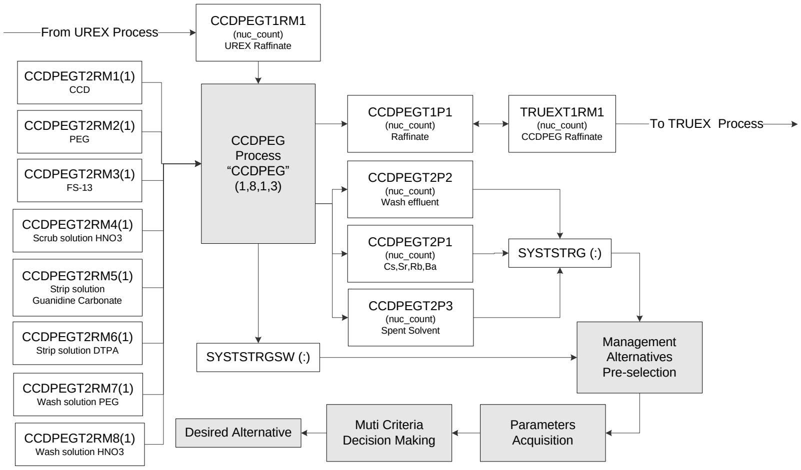

Figure C-6a CCDPEG process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed

(b) Steady state calculation with no loss due to third phase formation.

(c) Target separation efficiencies of all key elements are supplied by the AFC model.

(d) Cs, Sr, Rb and Ba are the only four elements that can be extracted into organic phase, hence no other nuclides presented in loaded solvent.

(e) Only one interested product stream which contains Cs, Sr, Rb and Ba in stripped product. Other elements remain in raffinate.

(f) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

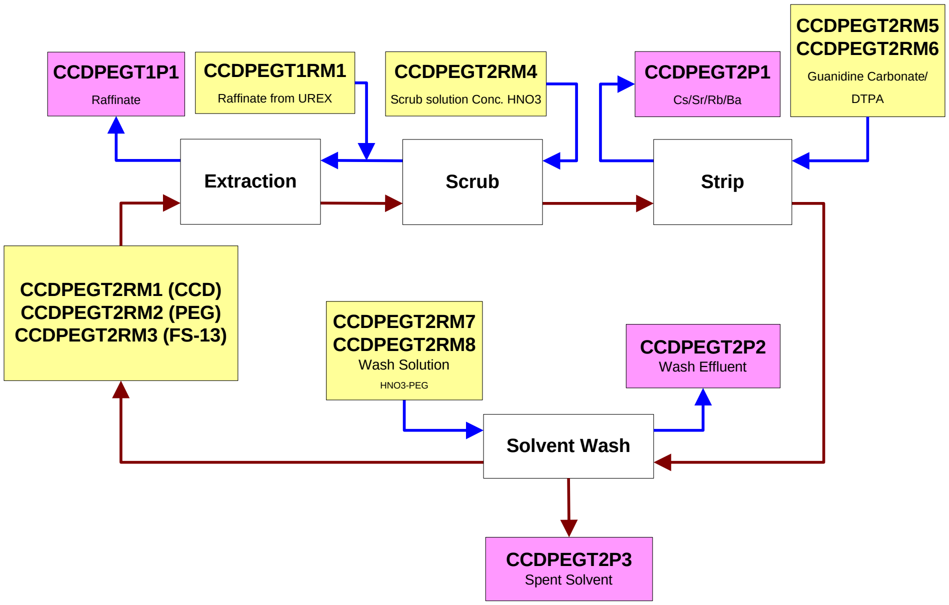

Figure C-6b CCDPEG process streams flow

Process descriptions:

(a) One input stream of type I—raffinate from UREX process with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via “UREX_BOX” subroutine.

(b) Eight input streams of type II (raw material), all of them are chemical reagent used in CCDPEG process.

(c) One output stream of type I —CCDPEG raffinate with maximum number of existing radionuclide in the stream equal nuc_count. This stream is determined via “CCDPEG_BOX” subroutine.

(d) Three output streams of type II— Cs/Sr.Rb/Ba product and solvent wash effluent with maximum number of existing radionuclide in all streams equal nuc_count. This stream is also determined via “CCDPEG_BOX” subroutine.

Mass balance:

Figure C-6a illustrates how mass balances of radionuclides distributed throughout CCDPEG process

TRUEX process

Process assumption:

(a) The Major calculation regarding TRUEX process was included in subroutines “TRUEX_BOX” inherited in module name “BOXROUTINES”.

(b) Required input information includes

(1) Input file name "truex_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed. Example of information in this input file are as followed; Steady state volumetric flow rate of each individual stream (input and output) of TRUEX process, needed for an estimation of reagents consumed in the process, was obtained from . Mass fraction of all

TRU elements distributed in wash effluent was obtained from the same document (if applicable otherwise they are assumed).

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "truex_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name “truex_cost.inp” that was created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

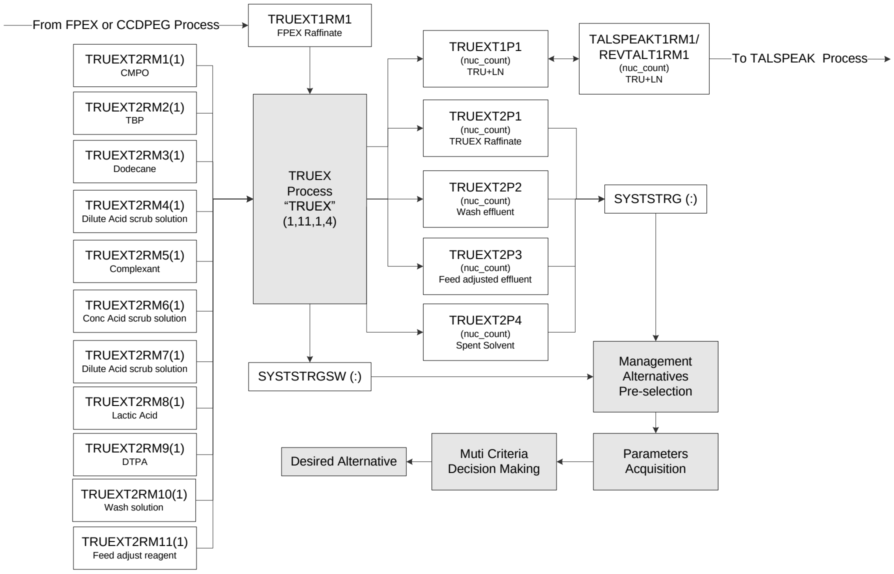

Figure C-7a TRUEX process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed

(b) Steady state calculation with no loss due to third phase formation.

(c) Target separation efficiencies of all key elements are supplied by the AFC model.

(d) In general, some of final extracted products involve more than single extraction cycle such as TRU and LN, which in reality each extraction cycle has its own recovery efficiency. Hence in this research, target efficiency for process segments (TRUEX, TALSPEAK, and etc) are assumed to be equal for involved process segments. For example if target separation efficiency for Cm is 99.99 percents, and there are two processes involved, TRUEX and TALSPEAK, the target efficiencies for both of them are equal square root of 99.99 percents which keeps the total the same.

(e) Only TRU and LN elements can be extracted into organic phase, hence no other nuclides besides TRUs and LNs presented in loaded solvent.

(f) Major fission products remain in raffinate.

(g) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

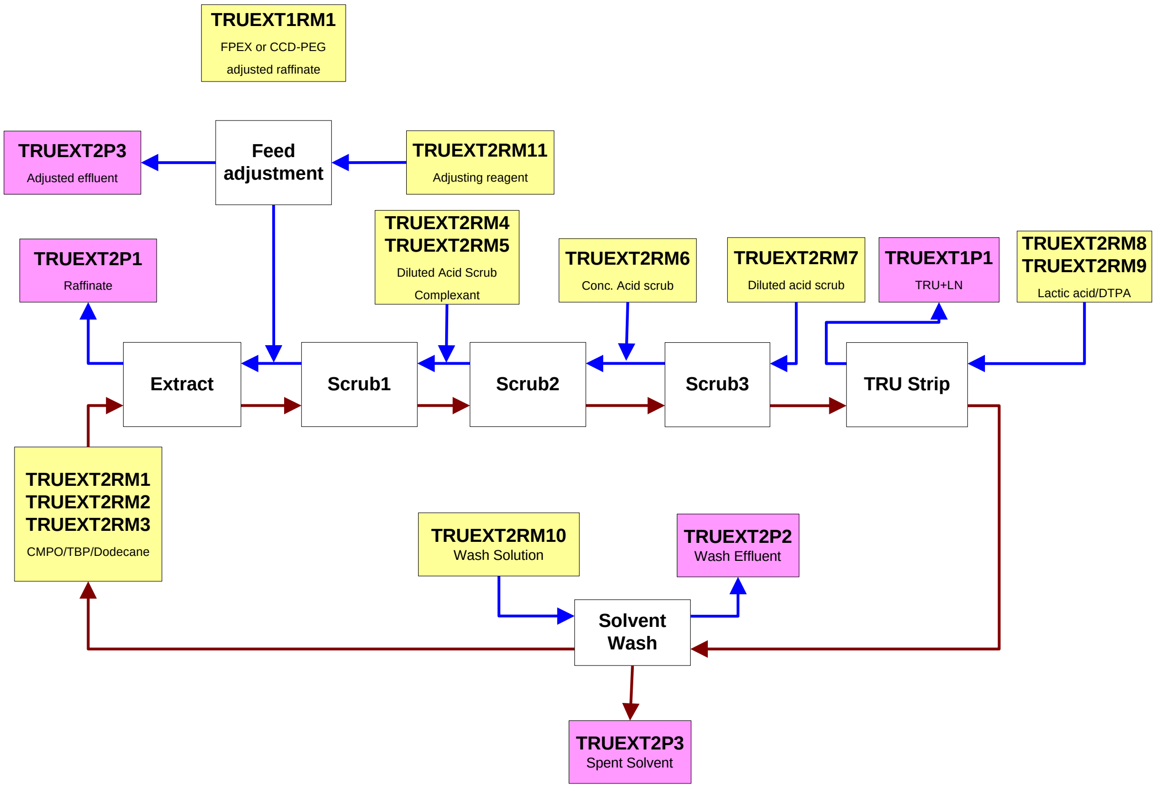

Figure C-7b TRUEX process streams flow

Process descriptions:

(a) One input stream of type I—raffinate from either FPEX or CCDPEG process with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via “TRUEX_BOX” subroutine.

(b) Eleven input streams of type II (raw material), all of them are chemical reagent used in TRUEX process.

(c) One output stream of type I —TRUEX loaded solvent with maximum number of existing radionuclide in the stream equal nuc_count. This stream is determined via “TRUEX_BOX” subroutine.

(d) Four output streams of type II—LNs product and solvent wash effluent with maximum number of existing radionuclide in all streams equal nuc_count and TRUEX feed adjustment effluent. These streams are also determined via “TRUEX_BOX” subroutine.

Mass balance:

Figure C-7a illustrates how mass balances of radionuclides distributed throughout TRUEX process

TALSPEAK process

Process assumption:

(a) The Major calculation regarding TALSPEAK process was included in subroutines "TALSPEAK_BOX" inherited in module name "BOXROUTINES".

(b) Required input information includes

(1) Input file name "talspeak_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed. Example of information in this input file are as followed; Steady state volumetric flow rate of each individual stream (input and output) of TALSPEAK process, needed for an estimation of reagents consumed in the process, was obtained from []. Mass fraction of all TRU elements distributed in wash effluent was obtained from the same document (if applicable otherwise they are assumed).

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "talspeak_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name "talspeak_cost.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

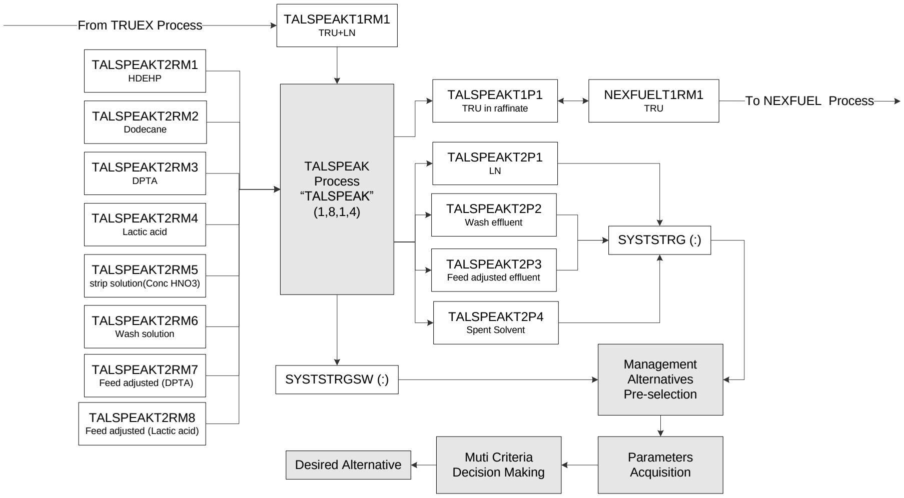

Figure C-8a TALSPEAK process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed

(b) Steady state calculation with no loss due to third phase formation.

(c) Target separation efficiencies of all key elements are supplied by the AFC model.

(d) In general, some of final extracted products involve more than single extraction cycle such as TRU and LN, which in reality each extraction cycle has its own recovery efficiency. Hence in this research, target efficiency for process segments (TRUEX, TALSPEAK, and etc) are assumed to be equal for involved process segments. For example if target separation efficiency for Cm is 99.99 percents, and there are two processes involved, TRUEX and TALSPEAK, the target efficiencies for both of them are equal square root of 99.99 percents which keeps the total the same.

(e) LN elements are extracted into organic phase, and stripped while TRUs are left behind in the raffinate. No other nuclides besides LNs presented in loaded solvent and also for solvent wash effluent.

(f) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

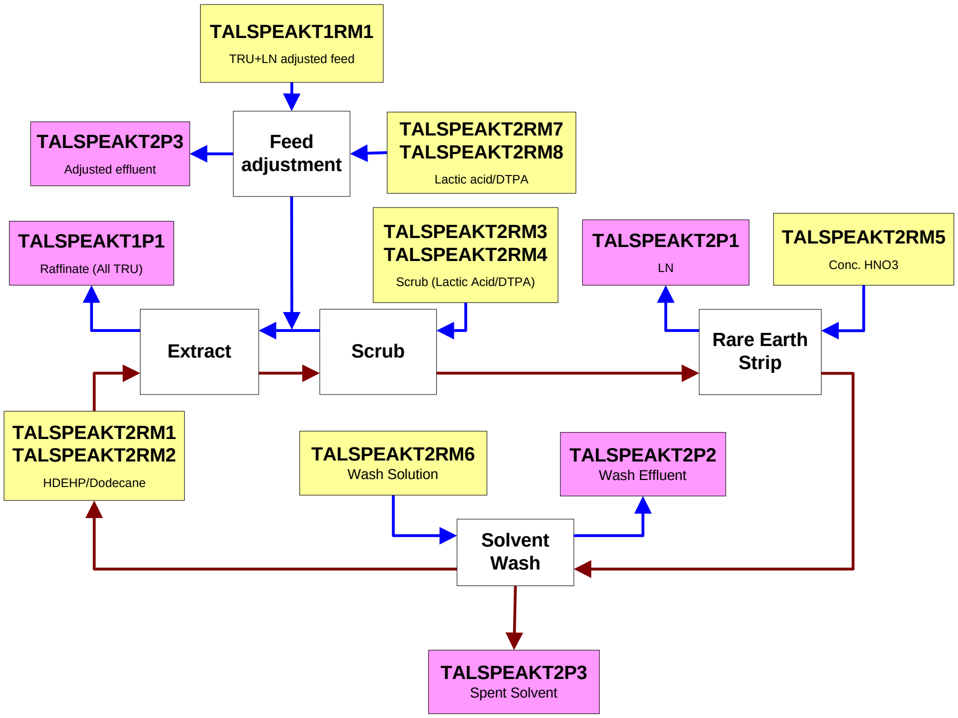

Figure C-8b TALSPEAK process streams flow

Process descriptions:

(a) One input stream of type I—TRUs and LNs in loaded solvent from TRUEX process, with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via "TALSPEAK_BOX" subroutine.

(b) Eight input streams of type II (raw material), all of them are chemical reagent used in TALSPEAK process.

(c) One output stream of type I — TRU products (in raffinate) with maximum number of existing radionuclide in the stream equal nuc_count. This stream is determined via "TALSPEAK_BOX" subroutine.

(d) Four output streams of type II— LNs stripped product and solvent wash effluent with maximum number of existing radionuclide in all streams equal nuc_count and TALSPEAK feed adjustment effluent. These streams are also determined via "TALSPEAK _BOX" subroutine.

Mass balance:

Figure C-8a illustrates how mass balances of radionuclides distributed throughout TALSPEAK process

Reversed TALSPEAK process

Process assumptions:

(a) The Major calculation regarding TALSPEAK process was included in subroutines "TALSPEAK_BOX" inherited in module name "BOXROUTINES".

(b) Required input information includes:

(1) Input file name "revtal_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed. Example of information in this input file are as followed; Steady state volumetric flow rate of each individual stream (input and output) of reversed TALSPEAK process, needed for an estimation of reagents consumed in the process, was obtained from []. Mass fraction of all TRU elements distributed in wash effluent was obtained from the same document (if applicable otherwise they are assumed)

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "revtal_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name “revtal_cost.inp” that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

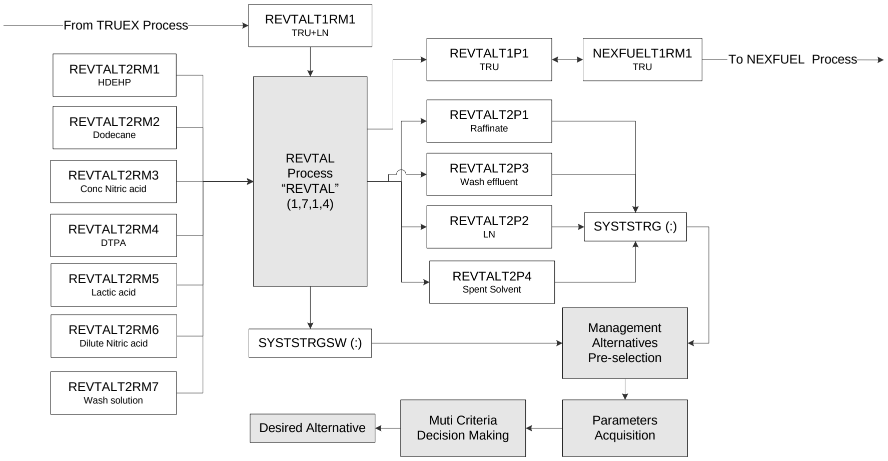

Figure C-9a Reversed TALSPEAK process flow diagram Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed.

(b) Steady state calculation with no loss due to third phase formation.

(c) Target separation efficiencies of all key elements are supplied by the AFC model.

(d) In general, some of final extracted products involve more than single extraction cycle such as TRU and LN, which in reality each extraction cycle has its own recovery efficiency. Hence in this research, target efficiency for process segments (TRUEX, TALSPEAK, and Reversed TALSPEAK) are assumed to be equal for involved process segments. For example if target separation efficiency for Cm is 99.99 percents, and there are two processes involved, TRUEX and TALSPEAK, the target efficiencies for both of them are equal square root of 99.99 percents which keeps the total the same.

(e) Both TRUs and LNs are extracted into organic phase, and simultaneous stripped into separated streams while trace TRUs and LNs are left behind in the raffinate. No other nuclides besides TRUs and LNs presented in loaded solvent and also for solvent wash effluent.

(f) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

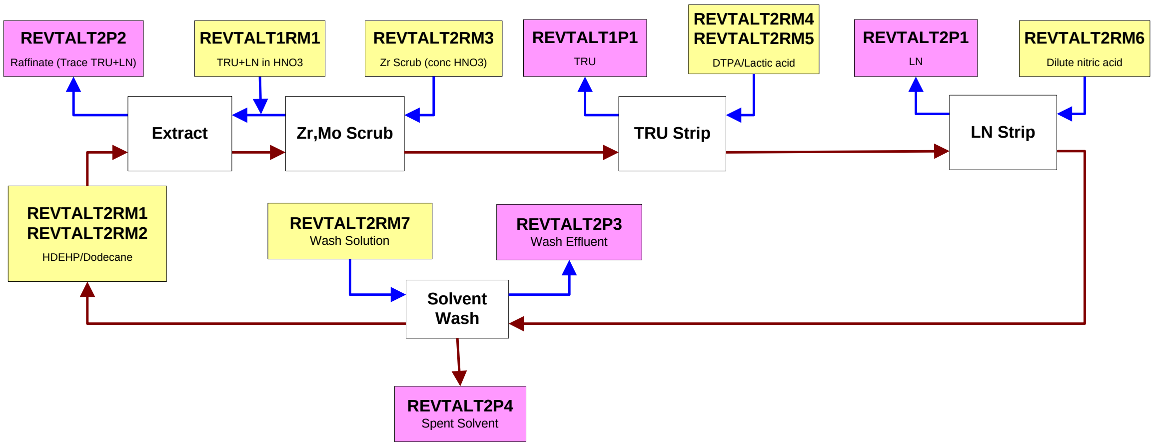

Figure C-9b Reversed TALSPEAK process streams flow

Process descriptions:

(a) One input stream of type I—TRUs and LNs in loaded solvent from TRUEX process, with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via “REVTAL_BOX” subroutine.

(b) Seven input streams of type II (raw material), all of them are chemical reagent used in reversed TALSPEAK process.

(c) One output stream of type I — TRU products (in stripped product) with maximum number of existing radionuclide in the stream equal nuc_count. This stream is determined via “REVTAL_BOX” subroutine.

(d) Four output streams of type II— LNs stripped product and solvent wash effluent with maximum number of existing radionuclide in all streams equal nuc_count and reversed TALSPEAK raffinate. These streams are also determined via “REVTAL _BOX” subroutine.

Mass balance:

Figure C-9a illustrates how mass balances of radionuclides distributed throughout reversed TALSPEAK process.

MOXFUEL process

Process assumptions:

(a) The Major calculation regarding MOX fuel fabrication process was included in subroutines “MOXFUEL _BOX” inherited in module name “BOXROUTINES”.

(b) The system process box combine two actual processes; conversion and fabrication into a simple process modeling box.

(c) Required input information includes

(1) Input file name "moxfuel_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed.

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "moxfuel_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name “moxfuel_cost.inp” that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

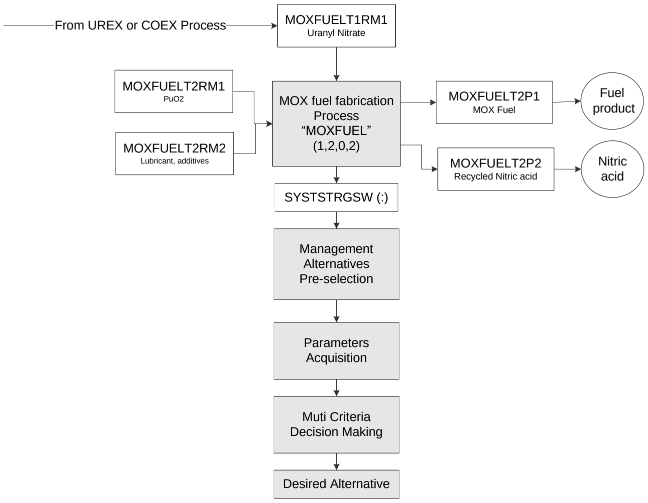

Figure C-10a Mixed Oxide fuel fabrication process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed

(b) Steady state calculation with no loss due to third phase formation.

(c) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

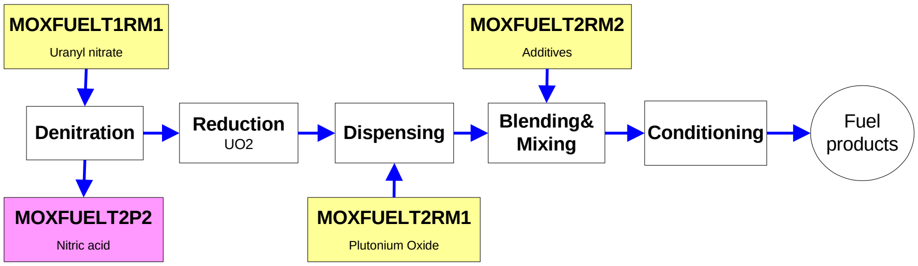

Figure C-10b Mixed Oxide fuel fabrication process streams flow

Process descriptions:

(a) One input stream of type I—U products from either UREX or COEX process, with maximum number of existing radionuclide in the stream equal nuc_count. This stream is calculated internally in IWMS model via “UREX_BOX” or “COEX_BOX” subroutines.

(b) Two input streams of type II (raw material), all of them are chemical reagent used in reversed TALSPEAK process.

(c) There is no output stream of type I for MOX fuel fabrication process.

(d) Two output streams of type II— MOX fuel product and nitric acid.These streams are determined via “MOXFUEL _BOX” subroutines.

Mass balance:

Figure C-10a illustrates how mass balances of radionuclides distributed throughout the process.

NEXFUEL process

Process assumptions:

(a) The Major calculation regarding Next generation fuel fabrication process was included in subroutines “NEXFUEL_BOX” inherited in module name “BOXROUTINES”.

(b) The system process box combine two actual processes; conversion and fabrication into a simple process modeling box.

(c) Required input information includes:

(1) Input file name "nexfuel_box.inp" created by macro function in Excel spreadsheet and then imported into subroutines when needed.

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name "nexfuel_sw.inp" that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name “nexfuel_cost.inp” that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

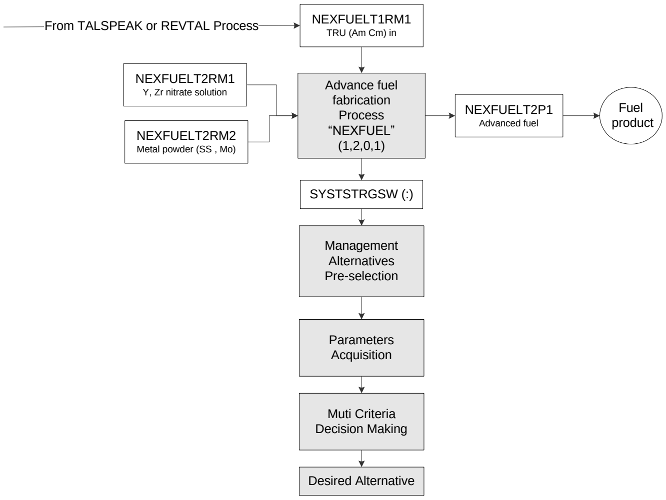

Figure C-11a Next generation fuel fabrication process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed.

(b) Steady state calculation with no loss due to third phase formation.

(c) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

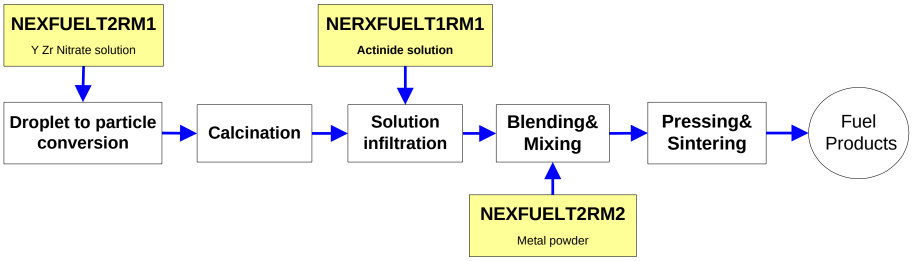

Figure C-11b Next generation fuel fabrication process streams flow

Process descriptions:

(a) One input stream of type I—TRU products from either TALSPEAK or Reversed TALSPEAK process. This stream is calculated internally in IWMS model via“TALSPEAK_BOX” or “REVTAL_BOX” subroutines.

(b) Two input streams of type II (raw material), all of them are chemical reagent used in MOX fuel fabrication process.

(c) There is no output stream of type I for next generation fuel fabrication process.

(d) One output stream of type II— Next generation fuel product which is determined via “NEXFUEL_BOX” subroutines.

Mass balance:

Figure C-11a illustrates how mass balances of radionuclides distributed throughout the process.

OFGT process

Process assumption:

(a) The Major calculation regarding Next generation fuel fabrication process was included in subroutines “OFGTC_BOX” or “OFGTV_BOX” inherited in module name “BOXROUTINES”.

(b) Required input information includes

(1) Input file name “ofgtc_box.inp” or “ofgtv_box.inp” (depend on voloxidation process is employed or not) created by macro function in Excel spreadsheet and then imported into subroutines when needed.

(2) Other process parameters specified inside the procedure themselves.

(3) Radioactive waste associated with the process, which is included in the input file name “ofgtc_sw.inp” or “ofgtv_sw.inp” that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

(4) Costs associated with the process, which is included in the input file name “ofgtc_cost.inp” or “ofgtv_cost.inp” that is created by macro execution in Excel spreadsheet and then imported into the subroutines when needed.

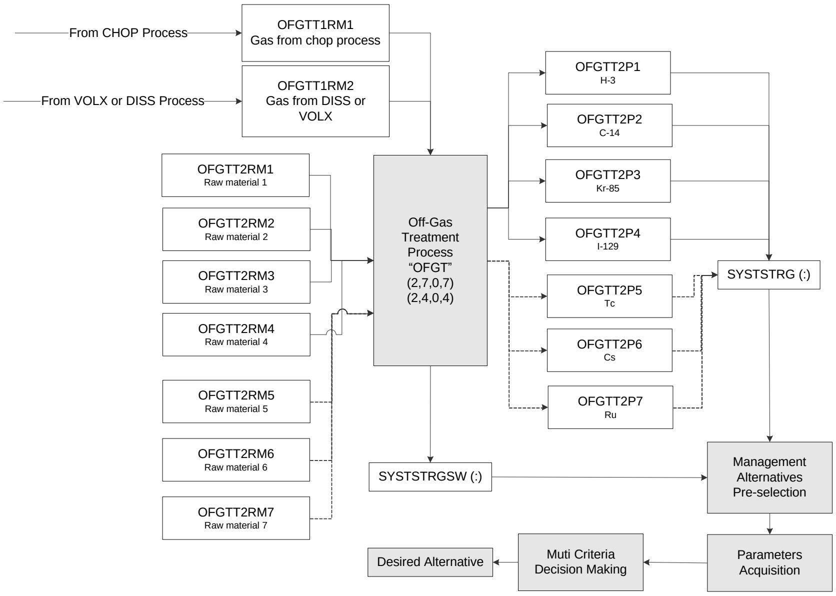

Figure C-12 Off-Gas Treatment process flow diagram

Assumptions:

(a) Simple mass balance calculation throughout the process segment was assumed

(b) Steady state calculation with no loss due to third phase formation.

(c) Contamination fraction (F_SW) for all radionuclides is the same. The secondary wastes type (i.e. metal, ash, resin, equipment) were fixed but the fraction of radioactivity that contributes to each type depend on the process obtained during the process.

Process descriptions:

(For OFGTC)

(a) Two input streams of type I—FPs gas from chopping and dissolution processes. These streams are calculated internally in IWMS model via "CHOP_BOX" and "DISSC_BOX" subroutines respectively.

(b) Four input streams of type II (raw material)—can be key raw materials of FP gas decontamination technologies

(c) There is no output stream of type I.

(d) Four output streams of type II—C-14, H-3, I-129, and Kr-85 streams. These streams are determined via "OFGTC_BOX" subroutine.

Process descriptions:

(For OFGTV)

(a) Two input streams of type I—FPs gas from chopping and voloxidation processes. These streams are calculated internally in IWMS model via "CHOP_BOX" and "VOLX_BOX" subroutines respectively.

(b) Six input streams of type II (raw material) —can be key raw materials of FP gas decontamination technologies

(c) There is no output stream of type I.

(d) Six output streams of type II—C-14, H-3, I-129, Kr-85, Cs, Tc and Ru streams. These streams are determined via “OFGTV_BOX” subroutine

Mass balance:

Figure C-12 illustrates how mass balances of radionuclides distributed throughout off-gas treatment process (when voloxidation is and is not considered) are determined.

Appendix D IWMS Input and output files locations

All IWMS relevant input and output files are located in folder “C:\IWMS\Code\”. The following provides location for these files.

C:\IWMS\Code\IWMS.xlsx
C:\IWMS\Code\IWMS_main.exe
C:\IWMS\Code\IWMS_boxroutinesmodule.f90
C:\IWMS\Code\IWMS_classroutinesmodule.f90
C:\IWMS\Code\IWMS_dcalculateroutinesmodule.f90
C:\IWMS\Code\IWMS_doseroutinesmodule.f90
C:\IWMS\Code\IWMS_driverroutinesmodule.f90
C:\IWMS\Code\IWMS_groundtransportroutinesmodule.f90
C:\IWMS\Code\IWMS_idcalculateroutinesmodule.f90
C:\IWMS\Code\IWMS_main.f90
C:\IWMS\Code\IWMS_makedecisionroutinesmodule.f90
C:\IWMS\Code\IWMS_mcdaroutinesmodule.f90
C:\IWMS\Code\IWMS_shareddatamodule.f90
C:\IWMS\Code\IWMS_subidcalculateroutinesmodule.f90
C:\IWMS\Code\IWMS_typesmodule.f90
C:\IWMS\Code\IWMS_wdrroutinemodule.f90
C:\IWMS\Code\call_scale.bat
C:\IWMS\Code\Input\

- C:\IWMS\Code\Input\
- C:\IWMS\Code\Input\GroundTransports
    - C:\IWMS\Code\Input\GroundTransports\Texas_sat.inp
    - C:\IWMS\Code\Input\GroundTransports\Texas_unsat.inp
    - C:\IWMS\Code\Input\GroundTransports\YMF_sat.inp
    - C:\IWMS\Code\Input\GroundTransports\YMF_unsat.inp
- C:\IWMS\Code\Input\Processbox
    - C:\IWMS\Code\Input\Processbox\Cost\
        - C:\IWMS\Code\Input\Processbox\Cost\ccdpeg_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\coex_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\fpex_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\moxfuel_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\nexfuel_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\ofgtc_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\ofgtv_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\revtal_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\talspeak_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\truex_cost.inp
        - C:\IWMS\Code\Input\Processbox\Cost\urex_cost.inp
    - C:\IWMS\Code\Input\ Processbox\ccdpeg_box.inp
    - C:\IWMS\Code\Input\ Processbox\chop_box.inp
    - C:\IWMS\Code\Input\ Processbox\coex_box.inp
    - C:\IWMS\Code\Input\ Processbox\diss1_box.inp
    - C:\IWMS\Code\Input\ Processbox\diss2_box.inp
    - C:\IWMS\Code\Input\ Processbox\fpex_box.inp
    - C:\IWMS\Code\Input\ Processbox\moxfuel_box.inp
    - C:\IWMS\Code\Input\ Processbox\nexfuel_box.inp
    - C:\IWMS\Code\Input\ Processbox\ofgtc_box.inp
    - C:\IWMS\Code\Input\ Processbox\ofgtv_box.inp
    - C:\IWMS\Code\Input\ Processbox\revtal_box.inp
    - C:\IWMS\Code\Input\ Processbox\talspeak_box.inp

  - C:\IWMS\Code\Input\ Processbox\truex_box.inp
  - C:\IWMS\Code\Input\ Processbox\urex_box.inp
  - C:\IWMS\Code\Input\ Processbox\volx_box.inp
- C:\IWMS\Code\Input\Swaste\
  - C:\IWMS\Code\Input\Swaste\ccdpeg_sw.inp
  - C:\IWMS\Code\Input\Swaste\chop_sw.inp
  - C:\IWMS\Code\Input\Swaste\coex_sw.inp
  - C:\IWMS\Code\Input\Swaste\disb_sw.inp
  - C:\IWMS\Code\Input\Swaste\dissc_sw.inp
  - C:\IWMS\Code\Input\Swaste\dissv_sw.inp
  - C:\IWMS\Code\Input\Swaste\fpex_sw.inp
  - C:\IWMS\Code\Input\Swaste\moxfuel_sw.inp
  - C:\IWMS\Code\Input\Swaste\nexfuel_sw.inp
  - C:\IWMS\Code\Input\Swaste\ofgtc_sw.inp
  - C:\IWMS\Code\Input\Swaste\ofgtv_sw.inp
  - C:\IWMS\Code\Input\Swaste\revtal_sw.inp
  - C:\IWMS\Code\Input\Swaste\talspeak_sw.inp
  - C:\IWMS\Code\Input\Swaste\truex_sw.inp
  - C:\IWMS\Code\Input\Swaste\urex_sw.inp
  - C:\IWMS\Code\Input\Swaste\volx_sw.inp
- C:\IWMS\Code\Input\Wasteforms\
  - C:\IWMS\Code\Input\Wasteforms\ceramic.inp
  - C:\IWMS\Code\Input\Wasteforms\concrete.inp
  - C:\IWMS\Code\Input\Wasteforms\disposal.inp
  - C:\IWMS\Code\Input\Wasteforms\glass.inp
  - C:\IWMS\Code\Input\Wasteforms\metal.inp
  - C:\IWMS\Code\Input\Wasteforms\polymer.inp
  - C:\IWMS\Code\Input\Wasteforms\VR.inp
- C:\IWMS\Code\Input\cladinv.inp
- C:\IWMS\Code\Input\costbox.inp
- C:\IWMS\Code\Input\fpinv.inp
- C:\IWMS\Code\Input\indices.dat
- C:\IWMS\Code\Input\pdcflib.dat
- C:\IWMS\Code\Input\recovery_eff.inp
- C:\IWMS\Code\Input\structinv.inp
- C:\IWMS\Code\Input\sub_weight.inp
- C:\IWMS\Code\Input\table1.inp
- C:\IWMS\Code\Input\table2.inp
- C:\IWMS\Code\Input\top_weight.inp
- C:\IWMS\Code\Input\wdr.dat

C:\IWMS\Code\Output\

- C:\IWMS\Code\Output\
  - C:\IWMS\Code\Output\Check\
    - C:\IWMS\Code\Output\Check\ccdpeg_check.out
    - C:\IWMS\Code\Output\Check\ccdpeg_check1.out
    - C:\IWMS\Code\Output\Check\chop_check.out
    - C:\IWMS\Code\Output\Check\chop_check1.out
    - C:\IWMS\Code\Output\Check\coex_check.out
    - C:\IWMS\Code\Output\Check\coex_check1.out
    - C:\IWMS\Code\Output\Check\disb_check.out
    - C:\IWMS\Code\Output\Check\disb_check1.out
    - C:\IWMS\Code\Output\Check\dissc_check.out
    - C:\IWMS\Code\Output\Check\dissc_check1.out
    - C:\IWMS\Code\Output\Check\dissv_check.out
    - C:\IWMS\Code\Output\Check\dissv_check1.out
    - C:\IWMS\Code\Output\Check\fpex_check.out

    - C:\IWMS\Code\Output\Check\fpex_check1.out
    - C:\IWMS\Code\Output\Check\moxfuel_check.out
    - C:\IWMS\Code\Output\Check\moxfuel_check1.out
    - C:\IWMS\Code\Output\Check\nexfuel_check.out
    - C:\IWMS\Code\Output\Check\nexfuel_check1.out
    - C:\IWMS\Code\Output\Check\ofgtc_check.out
    - C:\IWMS\Code\Output\Check\ofgtc_check1.out
    - C:\IWMS\Code\Output\Check\ofgtv_check.out
    - C:\IWMS\Code\Output\Check\ofgtv_check1.out
    - C:\IWMS\Code\Output\Check\revtal_check.out
    - C:\IWMS\Code\Output\Check\revtal_check1.out
    - C:\IWMS\Code\Output\Check\talspeak_check.out
    - C:\IWMS\Code\Output\Check\ccdpeg_check1.out
    - C:\IWMS\Code\Output\Check\talspeak_check1.out
    - C:\IWMS\Code\Output\Check\truex_check.out
    - C:\IWMS\Code\Output\Check\truex_check1.out
    - C:\IWMS\Code\Output\Check\urex_check.out
    - C:\IWMS\Code\Output\Check\urex_check1.out
    - C:\IWMS\Code\Output\Check\sysoutput_check.out
- C:\IWMS\Code\Output\Code.out
- C:\IWMS\Code\Output\Cost.out
- C:\IWMS\Code\Output\DS.out
- C:\IWMS\Code\Output\DStrmoutput.out
- C:\IWMS\Code\Output\index.out
- C:\IWMS\Code\Output\IStrmoutput.out
- C:\IWMS\Code\Output\SWbyprocess.out
- C:\IWMS\Code\Output\SWbytype.out
- C:\IWMS\Code\Output\Sysoutput.out
- C:\IWMS\Code\Output\wdr.out
- C:\IWMS\Code\Output\wdr.sum

C:\IWMS\Code\Origen\

- C:\IWMS\Code\Origen\Clad_original.inp
- C:\IWMS\Code\Origen\Clad_original_wtimeplt.inp
- C:\IWMS\Code\Origen\Fuel_original.inp
- C:\IWMS\Code\Origen\Fuel_original_wtimeplt.inp
- C:\IWMS\Code\Origen\SS_original.inp
- C:\IWMS\Code\Origen\SS_original_wtimeplt.inp

Appendix E List of input parameters located in FORTRAN source code

The majority of the FORTRAN input parameters code is located in module “shareddata”, where these parameters were made available publicly. Other parameters are scattered between the modules that are related to their categories. These modules are shown as follow:

```
MODULE SHAREDDATA
USE TYPES
IMPLICIT NONE
SAVE
!*************************************************************************
! Common paramerters using in between head-end process calculations
! Most of data was taken from Turkey Point3 D15 fuel. All data was normalized to 1 MTU.
!*************************************************************************
        ! Data taken from literature
        REAL(KIND=8),PARAMETER::FP_GAS_REL=3.179D-2             ! Fission gas released in Litre/MWD Burnup
        REAL(KIND=8),PARAMETER::FUEL_RHO=1.097D1                ! Density of fuelmeat(UO2) (kgUO2/LUO2)
        REAL(KIND=8),PARAMETER::CLAD_RHO=6.44D0                 ! Density of fuel clad (kgclad/Lclad)
        REAL(KIND=8),PARAMETER::MET_RHO=7.9D0                   ! Density of structure materials (kgss/Lss)
        REAL(KIND=8),PARAMETER::MW_U=0.238D0                    ! Molecular weight of uranium (kg)
        REAL(KIND=8),PARAMETER::MW_HNO3=6.3012D-2               ! Molecular weight of nitric acid(kg)
        REAL(KIND=8),PARAMETER::SG_HNO3=1.5D0                   ! Specific gravity of nitric acid (no unit), 1.5 time water density at certain temperature
        REAL(KIND=8),PARAMETER::CONC_HNO3=0.985D0               ! Concentration (by weight) of nitric acid (no unit), 98.5 percent
        REAL(KIND=8),PARAMETER::FEED_DENSITY=1.2D0              ! Feed density (kg/L)
        REAL(KIND=8),PARAMETER::FEED_CONC=0.377D-3              ! U content in 1 Litre of feed solution 377 gU/L find reference
        REAL(KIND=8),PARAMETER::SPNT_SOLV_FRAC=1.D-1            ! Spent solvent volume fraction that can not be recycled and will be subjected to be waste
        ! Data derived from literature or calculation
        REAL(KIND=8),PARAMETER::FP_VOL_V=1.96218D0              ! Volume of FP gas total (L/MTU) @ 28.15 MWD/Assembly burnup-Turkey point fuel
        REAL(KIND=8),PARAMETER::FUEL_VOL=1.03549D2              ! Volume of fuel meat(UO2) (LUO2/MTU)
        REAL(KIND=8),PARAMETER::CLAD_VOL=3.52D1                 ! Volume of fuel clad (Lclad/MTU)
        REAL(KIND=8),PARAMETER::MET_VOL=3.58D0                  ! Volume of structure materials (Lss/MTU)
        ! Makeup or assumed data
        REAL(KIND=8),PARAMETER::POWDER_VOL_F=1.D0               ! Volume of fuel powder produced from 1 litre fuel (Lpwd/LUO2)--MAKEUP DATA
        REAL(KIND=8),PARAMETER::POWDER_RHO=1.D1                 ! Density of fuel powder (kgpwd/Lpwd)      --MAKEUP DATA
        REAL(KIND=8),PARAMETER::FP_VOL_S=0.5D0                  ! Volume of FP gas contributed from semivolatile elements(Cs,Tc) total (L/MTU)
        REAL(KIND=8),PARAMETER::NDS_RHO=2.D0                    ! Density of Non-dissolved solid  (kgnds/Lnds)  --MAKEUP DATA
        REAL(KIND=8),PARAMETER::NDS_F=2.D-4                     ! Fraction of Non-dissolved solid per 1 litre of UO2  (LNDS/LUO2)  --MAKEUP DATA
        REAL(KIND=8),PARAMETER::FIVEYEAR=1.5768E8               ! 5 years limit in second; Cut off time to determine the class in LLW classification
        REAL(KIND=8),PARAMETER::T12_LIMIT=1.5768D8              ! (sec) Half-life segregation values to determine TRU waste classification
        REAL(KIND=8),PARAMETER::RNT_TO_RAD=0.877d0              ! Conversion factor for Roentgen/Rad
        REAL(KIND=8),PARAMETER::BQPERCI = 3.7D10                ! Conversion factor for Bq/Ci
        REAL(KIND=8),PARAMETER::STRG_TIME=9.46728D9             !(sec) Maximum allowable time of 300 years to store the stream represents reasonable
institutional control time
        REAL(KIND=8),PARAMETER::DOSELIMIT=0.5D0                 ! Intruder dose limit (rem) set by Section 3116, NDAA 2005 is 500 mrem
        REAL(KIND=8),PARAMETER::CONSMP_RATE = 0.51D0            ! Water consumption rate for human per year (m^3/year) RESRAD-offsite[67]
        REAL(KIND=8),PARAMETER::LN2 = 0.69314718D0
        REAL(KIND=8),PARAMETER::PI = 22.D0/7.D0

        ! Data for stream exempt
        CHARACTER(LEN=8),DIMENSION(150),PARAMETER::ISO_LIST=(/'Ac227','Ag108m','Am239','Am240','Am241', &
                'Am242','Am242m','Am243','Am244','Am244m','Am245','Am246','Ba133','Ba140','Ba141','Bi209','Bk249','C14','Cd109','Cd113m',  &
                'Ce144','Cf249','Cf250','Cf251','Cf252','Cl36','Cm241','Cm242','Cm243','Cm244','Cm245','Cm246','Cm247','Cm248','Cm249',  &
                'Cm250','Cm251','Co58','Co60','Cs134','Cs134m','Cs135','Cs136','Cs137','Cs140','Cs141','Cs142','Cs143','Cs144','Cs145',           &
                'Cs147','Eu149','Eu152','Eu154','Eu155','Eu156','Fe55','Fe59','H3','He4','Ho166m','I129','Kr85','Mn54','Mo93',  &
                'Nb91','Nb92','Nb93m','Nb94','Nb95','Nb95m','Ni59','Ni63','Np235','Np236','Np236m','Np237','Np238','Np239','Np240',  &
                'Np240m','Np241','Pa231','Pb206','Pb207','Pb208','Pb210','Pd107','Pm146','Pm147','Pu236','Pu237','Pu238','Pu239','Pu240',  &
                'Pu241','Pu242','Pu243','Pu244','Pu246','Ra226','Ra228','Rh102','Ru106','Sb124','Sb124m','Sb125','Sb126','Se79','Sm145',           &
                'Sm146','Sm148','Sm151','Sm155','Sn117m','Sn119m','Sn121','Sn121m','Sn123','Sn125','Sn125m','Sn126','Sr103','Sr87m','Sr89', &
                'Sr90','Sr91','Sr93','Sr95','Sr99','Tc98','Tc99','Te125m','Th228','Th229','Th230','Th232','U232','U233','U234',  &
                'U235','U236','U237','U238','V49','Y90','Y91','Y93','Zr93','Zr95' /)                    ! Available isotope list
```

```
        INTEGER,DIMENSION(150),PARAMETER::CHN_ID=(/3,0,3,4,1,2,2,3,4,4,1,2,0,6,7,0,1,0,0,0,0,1,2,3,4,0,1,2,3,4,1,2,3,4,1,2,3,0,0,0,0,0, &
                0,0,6,7,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,3,4,4,1,2,3,4,4,1,3,0,0,0,0,0,0,0,5,1,2,3,4,1,2,3,4,2,2,4,0,0, &
                0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,5,1,2,4,5,1,2,3,4,1,2,0,0,0,0,0,0  /)

        REAL(KIND=8),DIMENSION(150),PARAMETER::CLRNCE_LEVEL= (/2.0000D-02, 6.1668D-01, 3.9277D+00, 9.7327D-01, 3.0000D-01, 2.7624D+01, 3.0000D-01,
3.0000D-01, 1.1918D+00, 6.1641D+02, 1.6420D+01, 9.6358D-01, 2.4608D+00, 4.6926D+00, 1.0854D+00, &
        9.9900D+10, 1.0000D+02, 3.0000D+02, 3.0000D+02, 9.0000D+00, 3.0000D+01, 2.0000D-01, 4.0000D-01, 2.0000D-01, 5.0000D-01, 3.0000D+02, 1.9531D+00,
6.0000D+00, 4.0000D-01, 3.0000D-01, &
        3.0000D-01, 3.0000D-01, 3.0000D-01, 8.0000D-02, 2.1097D+01, 1.0000D-02, 2.1477D+00, 3.0000D+00, 3.0000D-01, 3.0000D-01, 2.6455D+01, 1.0000D+02,
5.3476D+01, 3.0000D-01, 5.0947D-01, &
        1.8799D-01, 1.3491D-01, 1.6312D-01, 1.1793D-01, 1.2627D-01, 1.8117D-01, 1.5569D+01, 3.0000D-01, 8.0077D-01, 1.4979D+01, 7.3964D-01, 3.0000D+02,
3.0000D+00, 3.0000D+03, 1.0000D-01, &
        5.7052D-01, 3.0000D+01, 3.6751D+01, 3.0000D-01, 8.8857D+01, 1.4327D+02, 6.3111D+00, 2.1053D+02, 3.0000D-01, 1.2980D+00, 1.1779D+01, 3.4904D+02,
3.0000D+03, 1.2285D+02, 1.0000D+00, &
        1.6835D+01, 3.0000D-01, 1.7361D+00, 5.0582D+00, 7.3438D-01, 2.5031D+00, 1.2061D+01, 1.0000D-01, 9.9000D+09, 9.9000D+09, 9.9000D+09, 3.0000D-01,
1.0417D+02, 1.3113D+00, 3.0000D+03, &
        7.0000D-01, 1.8560D+01, 3.0000D-01, 3.0000D-01, 3.0000D-01, 3.0000D+01, 3.0000D-01, 2.3474D+01, 3.0000D-01, 6.5617D+00, 3.0000D-01, 3.0000D-01, 4.6923D-
01, 3.0000D+00, 3.0000D-01, &
        2.7685D+00, 2.2731D+00, 3.4991D-01, 1.0000D+02, 1.4622D+01, 1.0000D+00, 1.0000D-02, 1.0000D+03, 6.3251D+00, 5.7438D+00, 5.1894D+01, 8.7719D+01,
1.1820D+02, 1.6984D+01, 2.5510D+00, &
        1.1882D+00, 1.3587D+01, 1.0000D-02, 3.0610D+00, 3.0000D+02, 3.0000D+00, 1.3184D+00, 9.6547D-01, 1.4350D-01, 1.2014D-01, 7.0131D-01, 3.0000D+02,
2.1552D+01, 3.0000D-01, 6.0000D-02, &
        3.0000D-01, 3.0000D-01, 1.0000D-01, 5.0000D-01, 3.0000D-01, 3.0000D-01, 6.0000D-01, 6.1958D+00, 3.0000D-01, 7.9177D+02, 3.0000D+02, 1.5672D+01,
4.8567D+00, 5.0000D+02, 1.3323D+00/)
        ! has unit of Bg/g -- IAEA-TECDOC-855 Clearance levels for radionuclides in solid materials,--[51] two more references are available but this is the most stringent one
        ! Data for Multi Criteria Decision Analysis
        REAL(KIND=8),DIMENSION(16),PARAMETER::w=(/6.25D-2,6.25D-2,6.25D-2,6.25D-2, &                    ! weight of importance of the jth criterion
          6.25D-2,6.25D-2,6.25D-2,6.25D-2,6.25D-2,6.25D-2,6.25D-2,6.25D-2,6.25D-2,6.25D-2,6.25D-2,6.25D-2 /)

        TYPE(ALTERN),PARAMETER::infras=ALTERN(1.D0,3.D0,5.D0,7.D0)             ! Default value for each alternative infrastructures, direct disposal, storage and
disposal, decontamination and recycle, and transmutation respectively (1 being most favorable) see derive type for detail
        TYPE(ALTERN),PARAMETER::practic=ALTERN(1.D0,3.D0,5.D0,7.D0)            ! Default value for each alternative practicality (7 being least favorable)
        ! Data for gamma exposure calculation, related to gamma energy bin from origen output
        REAL(KIND=8),DIMENSION(44),PARAMETER::Ebar=(/0.015D0,0.025D0,0.0375D0,0.0525D0,0.065D0,0.0725D0,0.0875D0, &
                0.125D0,0.175D0,0.23D0,0.28D0,0.35D0,0.425D0,0.48D0,0.511D0,0.556D0,0.65D0,0.75D0,   &
                0.85D0,0.95D0,1.1D0,1.265D0,1.385D0,1.47D0,1.535D0,1.615D0,1.73D0,1.9D0,2.075D0,   &
                2.25D0,2.425D0,2.625D0,2.875D0,3.25D0,3.75D0,4.25D0,4.75D0,5.25D0,5.75D0,6.25D0,   &
                6.75D0,7.25D0,7.75D0,9D0 /)
        REAL(KIND=8),DIMENSION(44),PARAMETER::Delta_E=(/0.015D0,0.01D0,0.0125D0,0.015D0,0.0125D0,0.0075D0,0.015D0, &
                0.0375D0,0.05D0,0.055D0,0.05D0,0.07D0,0.075D0,0.055D0,0.031D0,0.045D0,0.094D0,   &
                0.1D0,0.1D0,0.1D0,0.15D0,0.165D0,0.12D0,0.085D0,0.065D0,0.08D0,0.115D0,0.17D0,   &
                0.175D0,0.175D0,0.175D0,0.2D0,0.25D0,0.375D0,0.5D0,0.5D0,0.5D0,0.5D0,0.5D0,0.5D0,   &
                0.5D0,0.5D0,0.5D0,1.25D0 /)
        REAL(KIND=8),DIMENSION(44),PARAMETER::Mu_air=(/1.33400D+00,3.46300D-01,8.96725D-02,3.83375D-02,2.88250D-02,2.56550D-02, &
                2.34550D-02,2.41050D-02,2.58400D-02,2.72200D-02,2.82200D-02,2.91050D-02,2.95325D-02,2.96260D-02,2.96457D-02, &
                2.95885D-02,2.93525D-02,2.89975D-02,2.85875D-02,2.83085D-02,2.77916D-02,2.65648D-02,2.59936D-02,2.55985D-02, &
                2.53084D-02,2.49852D-02,2.45408D-02,2.38540D-02,2.32196D-02,2.27300D-02,2.22116D-02,2.16356D-02,2.09156D-02, &
                2.01025D-02,1.91675D-02,1.83750D-02,1.77250D-02,1.71675D-02,1.67025D-02,1.63175D-02,1.60125D-02,1.57075D-02, &
                1.54025D-02,1.48750D-02/)
                ! Mass Attenuation coefficient for air u_en/rho (cm^2/g), Reference from NIST database --RefWork ID 284 [58 ,96]

        ! Decay chain #1 data
        CHARACTER(LEN=6),DIMENSION(14),PARAMETER::CHN1_NAME                                                     =
(/'Cm249','Bk249','Cf249','Cm245','Pu241','Am241','Np237','U233','Th229','Am245','Np241','Cm241','U237','Pu237'/)
        INTEGER,DIMENSION(14),PARAMETER::CHN1_HEAD = (/0,1,2,3,4,5,6,7,8,0,0,0,0,0/)
        INTEGER,DIMENSION(14),PARAMETER::CHN1_TAIL = (/2,3,4,5,6,7,8,9,0,4,5,6,7,8/)
        INTEGER,DIMENSION(14),PARAMETER::CHN1_PARN = (/0,1,1,2,2,2,2,1,1,0,0,0,0,0/)
        REAL(KIND=8),DIMENSION(14),PARAMETER::CHN1_T12    =    (/1.2263D-4,0.876D0,3.5110D2,8.4987D3,1.43D1,4.33D2,2.14D6,1.59D5,7.34D3,2.34D-4,2.64D-
5,8.98D-2,1.85D-2,1.24D-1/)                                   ! Half-life in year

        ! Decay chain #2 data
        CHARACTER(LEN=6),DIMENSION(15),PARAMETER::CHN2_NAME                                                     =
(/'Cf250','Cm246','Pu242','U238','U234','Th230','Ra226','Am242','Am242m','Am246','Cm250','Pu246','Cm242','Pu238','Np238'/)
        INTEGER,DIMENSION(15),PARAMETER::CHN2_HEAD = (/0,1,2,3,4,5,6,0,0,0,0,0,0,0,0/)
        INTEGER,DIMENSION(15),PARAMETER::CHN2_TAIL = (/2,3,4,5,6,7,0,4,4,5,5,5,4,4,4/)
        INTEGER,DIMENSION(15),PARAMETER::CHN2_PARN = (/0,4,1,5,1,1,1,0,0,0,0,0,0,0,0/)
```

```
        REAL(KIND=8),DIMENSION(15),PARAMETER::CHN2_T12     =     (/15.D0,4.73D3,3.73D5,4.47D9,2.45D5,7.54D4,1.6D3,1.825D-3,1.41D2,4.75D-5,5.75D5,2.97D-
2,0.4461D0,8.7712D1,5.79603D-3/)                    ! Half-life in year

        ! Decay chain #3 data
        CHARACTER(LEN=6),DIMENSION(13),PARAMETER::CHN3_NAME                                                          =
(/'Cm251','Cf252','Am243','Pu239','U235','Pa231','Ac227','Pu243','Cm247','Am239','Cm243','Np239','Np235'/)
        INTEGER,DIMENSION(13),PARAMETER::CHN3_HEAD = (/0,1,2,3,4,5,6,0,0,0,0,0,0/)
        INTEGER,DIMENSION(13),PARAMETER::CHN3_TAIL = (/2,3,4,5,6,7,0,3,3,4,4,4,5/)
        INTEGER,DIMENSION(13),PARAMETER::CHN3_PARN = (/0,1,3,4,2,1,1,0,0,0,0,0,0/)
        REAL(KIND=8),DIMENSION(13),PARAMETER::CHN3_T12          =          (/3.1942D-5,2.65D0,7.3707D3,2.4111D4,7.03792D8,3.2759D4,2.1772D1,5.6537D-
4,1.5600D7,1.3575D-4,2.9099D1,6.45037D-3,1.0847D0/)              ! Half-life in year

        ! Decay chain #4 data
        CHARACTER(LEN=6),DIMENSION(15),PARAMETER::CHN4_NAME                                                          =
(/'Cf252','Cm248','Pu244','Pu240','U236','Th232','Ra228','Am240','Am244','Am244m','Cm244','Np240','Np240m','Np236','Np236m'/)
        INTEGER,DIMENSION(15),PARAMETER::CHN4_HEAD = (/0,1,2,3,4,5,6,0,0,0,0,0,0,0,0/)
        INTEGER,DIMENSION(15),PARAMETER::CHN4_TAIL = (/2,3,4,5,6,7,0,4,4,4,4,4,4,5,5/)
        INTEGER,DIMENSION(15),PARAMETER::CHN4_PARN = (/0,1,1,7,3,1,1,0,0,0,0,0,0,0,0/)
        REAL(KIND=8),DIMENSION(15),PARAMETER::CHN4_T12  =  (/2.6450D0,3.4799D5,7.9945D7,6.56D3,2.34206D7,1.4050D10,5.7461D0,5.79512D-3,1.15D-3,4.94D-
5,1.81D1,1.3727D-5,1.37D-5,1.53D5,2.57D-3/)                      ! Half-life in year

        ! Decay chain #5 data
        CHARACTER(LEN=6),DIMENSION(3),PARAMETER::CHN5_NAME = (/'Pu236', 'U232', 'Th228'/)
        INTEGER,DIMENSION(3),PARAMETER::CHN5_HEAD = (/0,1,2/)
        INTEGER,DIMENSION(3),PARAMETER::CHN5_TAIL = (/2,3,0/)
        INTEGER,DIMENSION(3),PARAMETER::CHN5_PARN = (/0,1,1/)
        REAL(KIND=8),DIMENSION(3),PARAMETER::CHN5_T12= (/2.87D+00,6.98D+01,1.91D0/)                    ! Half-life in year

        ! Decay chain #6 data
        CHARACTER(LEN=6),DIMENSION(2),PARAMETER::CHN6_NAME = (/'Cs140', 'Ba140'/)
        INTEGER,DIMENSION(2),PARAMETER::CHN6_HEAD = (/0,1/)
        INTEGER,DIMENSION(2),PARAMETER::CHN6_TAIL = (/2,0/)
        INTEGER,DIMENSION(2),PARAMETER::CHN6_PARN = (/0,1/)
        REAL(KIND=8),DIMENSION(2),PARAMETER::CHN6_T12= (/2.02D-6,3.4915D-2/)                ! Half-life in year

        ! Decay chain #7 data
        CHARACTER(LEN=6),DIMENSION(2),PARAMETER::CHN7_NAME = (/'Cs141', 'Ba141'/)
        INTEGER,DIMENSION(2),PARAMETER::CHN7_HEAD = (/0,1/)
        INTEGER,DIMENSION(2),PARAMETER::CHN7_TAIL = (/2,0/)
        INTEGER,DIMENSION(2),PARAMETER::CHN7_PARN = (/0,1/)
        REAL(KIND=8),DIMENSION(2),PARAMETER::CHN7_T12= (/7.87D-7,3.47D-5/)                  ! Half-life in year

        ! Alternative section parameters
        ! Parameter for Transmutation alternative (list for pre-decision and detail analysis)
        REAL(KIND=8),PARAMETER::FN=0.5D0              ! Utility fraction used for calculation of transmutation half-life— [54]
        REAL(KIND=8), PARAMETER::RQ_TAU = 2.D-1       ! Target transmutation halflife(Tau) (10 half time is 2 yrs irradiation of a target) — {{317 Bussard,R.W. 1993}}
        REAL(KIND=8),PARAMETER::YPERSEC=3.1689D-8     ! year per second
        TYPE(TRANSMUTE),PARAMETER::TRANSMUTE_LIST=TRANSMUTE( &                    ! All numerical data in this section need update
                ! List of nuclide in transmute list
                (/'I129','Tc99','Np237','Am241','Am243','Cm245','Cm246','Cm247','Cm248','Cm250'/), &

                ! Capability of being explicitly separated
                (/.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE./), &

                ! Cost of transmutation of a nuclide (USD per kg)
                (/1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3/), &

                ! Number of product nuclide after transmutation
                (/1,1,5,5,5,5,5,5,5,5/), &

                ! Mean effective half-life of the products (years)
                (/1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3/), &

                ! Relative toxicity of the daughters combined to the parents (less than 1.0 is preferred)
                (/0.5D0,0.5D0,0.6D0,0.5D0,0.5D0,0.5D0,0.5D0,0.5D0,0.5D0,0.5D0/), &

                ! Transmutation time taken to make the longest lived product to the clearance level (hours)
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```
            (/1.D4,1.D4,1.D4,1.D4,1.D4,1.D4,1.D4,1.D4,1.D4,1.D4/), &

            ! Combined properties that would make explicit separation condition be true, only liquid would satisfy the condition
            (/'LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID'/))

! Parameter for Decontamination and Recycle alternative (list for pre-decision and detail analysis)
TYPE(RECYCLE)::PARAMETER,RECYCLE_LIST=RECYCLE( &                                ! All numerical data in this section need update
            ! List of nuclide in transmute list
            (/'C14','Ce144','Eu149','Eu150','Eu154','Eu155','Eu156','H3','Ho166m','Kr85', &
              'Pm146','Pm147','Sm145','Sm146','Sm148','Sm151','Sm155'/), &

            ! Capability of being explicitly separated
            (/.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE., &
              .TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE./), &

            ! Cost to separate element (USD per kg)
            (/1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3, &
              1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3/), &

            ! Cost to separate isotope (USD per kg)
            (/1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3, &
              1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3/), &

            ! Profit made from a nuclide (USD per kg)
            ! Cost to recycle of a nuclide, include separation(USD per kg)
            (/1.5D3,1.1D3,1.1D3,1.2D3,1.3D3,1.3D3,1.2D3,1.5D3,1.5D3,1.5D3, &
              1.2D3,1.1D3,1.1D3,1.2D3,1.2D3,1.2D3,1.4D3/), &

            ! Major application for a nuclide
            (/'C14','Ce144','Eu149','Eu150','Eu154','Eu155','Eu156','H3','Ho166m','Kr85', &
              'Pm146','Pm147','Sm145','Sm146','Sm148','Sm151','Sm155'/), &

            ! Separation process for a particular nuclide
            (/'TOBEFILLED','SOLV_EXT','SOLV_EXT','SOLV_EXT','SOLV_EXT','SOLV_EXT','SOLV_EXT','TOBEFILLED','SOLV_EXT','CRYO', &
              'SOLV_EXT','SOLV_EXT','SOLV_EXT','SOLV_EXT','SOLV_EXT','SOLV_EXT','SOLV_EXT'/), &

            ! Combined properties that would make explicit separation condition be true, only liquid would satisfy the condition
            (/'TOBEFILLED','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','TOBEFILLED','LIQUID','CRYO', &
              'LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID','LIQUID'/), &

            ! Decontamination efficiency
            (/0.95D0,0.95D0,0.95D0,0.95D0,0.95D0,0.95D0,0.95D0,0.95D0,0.95D0,0.95D0, &
              0.95D0,0.95D0,0.95D0,0.95D0,0.95D0,0.95D0,0.95D0/))

! Parameter for Decay & Storage alternative (list for pre-decision and detail analysis)
REAL(KIND=8), PARAMETER::STORAGE_TIME = 1.5D2  ! Estimated storage time (years) for storage alternative
TYPE(STORAGE)::STORAGE_LIST=STORAGE( &
            ! List of nuclide in storage list
            (/'Cs134','Cs134m','Cs135','Cs136','Cs137','Cs140','Cs141','Cs142','Cs143','Cs144', &
              'Cs145','Cs147','Sr87m','Sr89','Sr90','Sr91','Sr93','Sr95','Sr99','Sr103'/), &

            ! Capability of a nuclide can adopt this alternative
            (/.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE., &
              .TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE.,.TRUE./), &

            ! Cost to store this nuclide (USD per kg)                          ! Costs need update --only have data for Dry cast storage for SNF
            (/1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3, &
              1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3,1.D3/), &

            ! Storage time taken to achieve clearance level
            (/1.D2,1.D2,1.D2,1.D2,1.D2,1.D2,1.D2,1.D2,1.D2,1.D2, &
             1.D2,1.D2,1.D2,1.D2,1.D2,1.D2,1.D2,1.D2,1.D2,1.D2/))

CHARACTER(LEN=6),DIMENSION(37),PARAMETER::POST_STRG_DAUG=(/'Ba133','Ba140','Ba141','Cs134','Cs135','Cs136','Cs137','Cs140','Cs141','Cs142', &
'Cs143','Cs144','Cs145','Cs147','Sr87m','Sr89','Sr90','Sr93','Sr95','Sr103','Cs133','Ce140','Pr141','Ba134','Ba135','Ba136','Ba137','Ce142','Nd143','Nd144',  &
'Nd145','Sm147','Sr87','Y89','Zr90','Zr93','Mo95' /)
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        CHARACTER(LEN=6),DIMENSION(37),PARAMETER::POST_STRG_PARE=(/'FP','FP','FP','FP','FP','FP','FP','FP','FP','FP', &
                'FP','FP','FP','FP','FP','FP','FP','FP','FP','FP','Ba133','Ba140','Ba141','Cs134','Cs135','Cs136','Cs137','Cs142','Cs143','Cs144',  &
                'Cs145','Cs147','Sr87m','Sr89','Sr90','Sr93','Sr95' /)

        ! Site parameters that are used in metal waste form source term calculations
        TYPE(SITEDATA_COMMON),PARAMETER::TEXAS_C=SITEDATA_COMMON( &                ! Common data for TEXAS site[l]
                ! Ph
                8.1D0,          &                       ! ACS data
                ! Temperature (Celsius)
                2.6D1,          &                       !
                ! Chlorine content at the facility (mg/L assume equivalent to ppm) ACS data--RefWork ID not available
                3.17D0)

        TYPE(SITEDATA_COMMON),PARAMETER::YMF_C=SITEDATA_COMMON( &                  ! Common data for YM site [m]
                ! Ph  --[83] (28-38 c p 825 UZ)
                8.1D0,          &
                ! Temperature (Celcius) --[83] (28-38 c p 1320 SZ)
                3.3D1,          &
                ! Chlorine content at the facility (mg/L assume equivalent to ppm)  --[83] (28-38 c p 825 UZ)
                6.8.D0)

        ! Source term related parameters
        REAL(KIND=8),PARAMETER::Fail_Time_Glass = 1.D3                  ! Time of Waste Package Failure for CSNF assumed to be the same for vitrified glass waste
package failure (y) Most reference use 1000 y package failure
        REAL(KIND=8),PARAMETER::Fail_Time_Metal_H = 1.D3                ! Time of Waste Package Failure for CSNF assumed to be the same for HLW metal waste
package failure (y)
        REAL(KIND=8),PARAMETER::Fail_Time_Metal_L = 0.D0                ! Time of Waste Package Failure for LLW assumed to be the same for LLW metal waste
package failure  (y)
        REAL(KIND=8),PARAMETER::Fail_Time_Concrete = 0.D0               ! Time of Waste Package Failure for LLW assumed to be the same for concrete waste form (y)
        REAL(KIND=8),PARAMETER::Fail_Time_Polymer = 0.D0                ! Time of Waste Package Failure for LLW assumed to be the same for polymer waste form (y)
        REAL(KIND=8),PARAMETER::Fail_Time_bitumen = 0.D0                ! Time of Waste Package Failure for LLW assumed to be the same for polymer waste form (y)

        REAL(KIND=8),PARAMETER::WS_PKG_vol = 0.25D0                     ! Volume of water in waste package (m^3)  --need update
        REAL(KIND=8),PARAMETER::qout = 0.5D0                            ! Rate at which water leave the waste package at time t-- assume constant (m^3/year)   --need
update

        TYPE(SOLUBDATA),PARAMETER::SOL_LIMIT = SOLUBDATA(&  ! Solubility limits of elements kg/m^3 use SKI Project 90 as reference --[85]
                ! List of element considered
                (/'Ac','Ag','Am','Ba','Bi','Bk','C','Cd','Ce','Cf', &
                'Cl','Cm','Co','Cs','Eu','Fe','H','He','Ho','I',     &
                'Kr','Mn','Mo','Nb','Ni','Np','Pa','Pb','Pd','Pm', &
                'Pu','Ra','Rh','Ru','Sb','Se','Sm','Sn','Sr','Tc',    &
                'Te','Th','U','V','Y','Zr' /),        &
                ! Solubility limit
   (/9.080000D-05,1.078700D-01,9.720000D-05,1.373300D-06,2.089600D-06, &
   2.470000D-06,1.201100D+02,1.124100D-03,1.401200D-06,2.510000D-06,3.545000D+02, &
   9.880000D-05,5.893000D+00,1.329100D-06,6.078400D-05,2.233800D-05,1.007000D+01, &
   4.002000D+01,6.597200D-05,1.269000D+03,8.380000D+02,2.197200D-05,9.594000D-01, &
   9.290600D-06,5.869000D+00,3.555000D-01,2.310400D-03,2.072000D-03,1.064200D-05, &
   5.800000D-05,7.320000D-03,9.040000D-05,4.116400D-05,4.042800D-05,4.870400D-05, &
   3.948000D+01,6.014400D-05,1.187100D-05,8.762000D-02,9.600000D+02,5.104000D-05, &
   5.104880D-06,3.570450D-01,9.400000D-06,3.556240D-05,9.122400D-08/))

END MODULE SHAREDDATA
```

Database in SUBROUTINE SAT_TRANSPORT

```
! Database for saturated zone in both HLW and LLW sites
TYPE(SITEDATA_SAT)::YMF=SITEDATA_SAT( &                                 ! YMF database for HLW disposal
! Distance of the exclusion zone (m)--Radionuclide transport simulation and uncertainty analyses with the saturated-zone site-scale model at Yucca Mountain, Nevada [62 ,97]
1.8D4,          &
! Hydraulic conductivity of the aquifer (m/yr) or (cm/s) ----input from excel[84]
4.38D3,         &
```

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[l] http://www.urs-slc.com/wcs/

[m] http://www.urs-slc.com/wcs/

```
! Water table slope in the direction to receptor location (m/m) -----[98] 3 different data are available but use moderata one
-1.5D-2,        &
! Porosity  --[84]
0.18D0,         &
! Effective porosity   ----input from excel --[84]
0.18D0,         &
! Bulk density (g/cm^3)          ----input from excel --[99]
1.27D0,         &
! List of element considered
(/'Ac','Ag','Am','Ba','Bi','Bk','C','Cd','Ce','Cf', &
'Cl','Cm','Co','Cs','Eu','Fe','H','He','Ho','I',      &
'Kr','Mn','Mo','Nb','Ni','Np','Pa','Pb','Pd','Pm', &
'Pu','Ra','Rh','Ru','Sb','Se','Sm','Sn','Sr','Tc',    &
'Te','Th','U','V','Y','Zr' /),        &
! Molecular diffusion coefficient (cm^2/s) EPA calculation method for diffusion coefficient-use water temp at 70 F--R [100] + data from two websites see excel (Molar Volumes were
taken from[n] and dynamic viscosities were taken from[o])
(/7.3896D-02, 1.1733D-01, 8.4993D-02, 5.3405D-02, 7.6262D-02, 8.8141D-02, 1.7308D-01, 1.0222D-01, 7.7161D-02, 8.8427D-02,  &
1.9250D-03, 8.3597D-02, 1.5207D-01, 3.7680D-02, 6.3734D-02, 1.4602D-01, 1.9069D-03, 1.2676D-03, 8.2356D-02, 6.8422D-02,  &
1.2700D-03, 1.4293D-01, 1.2422D-01, 1.1373D-01, 1.5250D-01, 1.0935D-01, 9.3817D-02, 8.3627D-02, 1.2816D-01, 7.9383D-02,  &
1.0551D-01, 4.9052D-02, 1.3343D-01, 1.3434D-01, 8.3873D-02, 8.9172D-02, 7.8262D-02, 8.9643D-02, 5.8708D-02, 1.3105D-01,  &
7.8262D-02, 7.9783D-02, 1.0461D-01, 1.3276D-01, 7.9571D-02, 9.7784D-02/), &
! Distribution coefficient,kd(mL/g)    ----input from excel--[86]
(/1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,              &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5/))

TYPE(SITEDATA_SAT)::TEXAS_S=SITEDATA_SAT( &                                    ! Saturated zone data for TEXAS site[p]
! Distance of the exclusion zone (m)
1.D3,           &
! Hydraulic conductivity of the aquifer (m/yr) or (cm/s)  ----input from excel
1.5D0,          &
! Water table slope in the direction to receptor location (m/m)
-1.5D-2,        &
! Porosity  ACS
0.15D0,         &
! Effective porosity   ----input from excel
0.1D0,          &
! Bulk density (g/cm^3)           ----input from excel
0.8D0,          &
! List of element considered
(/'Ac','Ag','Am','Ba','Bi','Bk','C','Cd','Ce','Cf', &
'Cl','Cm','Co','Cs','Eu','Fe','H','He','Ho','I',      &
'Kr','Mn','Mo','Nb','Ni','Np','Pa','Pb','Pd','Pm', &
'Pu','Ra','Rh','Ru','Sb','Se','Sm','Sn','Sr','Tc',    &
'Te','Th','U','V','Y','Zr' /),        &
! Molecular diffusion coefficient (cm^2/s)--ACS and EPA calculation method for diffusion coefficient-use viscosity data at 64.4 F
(/7.0248D-02, 1.1153D-01, 8.0797D-02, 5.0768D-02, 7.2496D-02, 8.3789D-02, 1.6453D-01, 9.7170D-02, 7.3351D-02, 8.4061D-02, &
1.8300D-03, 7.9470D-02, 1.4456D-01, 3.5820D-02, 6.0587D-02, 1.3881D-01, 1.8127D-03, 1.2050D-03, 7.8290D-02, 6.5044D-02, &
1.2073D-03, 1.3588D-01, 1.1809D-01, 1.0812D-01, 1.4497D-01, 1.0395D-01, 8.9185D-02, 7.9498D-02, 1.2183D-01, 7.5464D-02, &
1.0030D-01, 4.6630D-02, 1.2685D-01, 1.2771D-01, 7.9732D-02, 8.4769D-02, 7.4398D-02, 8.5217D-02, 5.5809D-02, 1.2458D-01, &
7.4398D-02, 7.5843D-02, 9.9442D-02, 1.2620D-01, 7.5643D-02, 9.2956D-02/), &

! Distribution coefficient,kd(mL/g)   ----input from excel
(/1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,              &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5/))
```

Database in SUBROUTINE UNSAT_TRANSPORT

```
! Some of these parameters are to be imported
TYPE(SITEDATA_UNSAT)::TEXAS_U=SITEDATA_UNSAT( &                                          ! Unsaturated zone data for TEXAS site
! Volumetric water content in unsaturated zone (m^3 water/m^3 soil) From ACS Table 6-4e Bore # B-46 Ground elevation 3470.19 below 50.0 sample elevation 3420.19 Silt clayey sand
4.89 percent
0.0489D0,      &
! Infiltration rate at the unsaturated zone disposal site  (m^3/y))----input from excel---need update
2.6D1,          &
! Bulk density (g/cm^3)  From ACS Table 6-4e Bore # B-46 Ground elevation 3470.19 below 50.0 sample elevation 3420.19 Silty clayey sand 4.89 percent
1.68D0,         &
! Depth to the acquifer (m) From the aquifer is found from 15 to 90 meters (50 to 300 feet) below the land surface
9.D1,           &
! Width of the disposal site (m) From estimated from 1338 acres of LLRW disposal area WCS website ACS
2.3269D3,      &
! Length of the disposal site (m) From estimated from 1338 acres of LLRW disposal area
2.3269D3,      &
```

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[n] http://periodictable.com/Properties/A/MolarVolume.html

[o] http://www.mhtl.uwaterloo.ca/old/onlinetools/airprop/airprop.html

[p] http://www.urs-slc.com/wcs/

```
! List of element considered
(/'Ac','Ag','Am','Ba','Bi','Bk','C','Cd','Ce','Cf', &
'Cl','Cm','Co','Cs','Eu','Fe','H','He','Ho','I',       &
'Kr','Mn','Mo','Nb','Ni','Np','Pa','Pb','Pd','Pm', &
'Pu','Ra','Rh','Ru','Sb','Se','Sm','Sn','Sr','Tc',    &
'Te','Th','U','V','Y','Zr' /),         &
! Molecular diffusion coefficient (cm^2/s)--ACS and EPA calculation method for diffusion coefficient-use viscosity data at 64.4 F
(/7.0248D-02, 1.1153D-01, 8.0797D-02, 5.0768D-02, 7.2496D-02, 8.3789D-02, 1.6453D-01, 9.7170D-02, 7.3351D-02, 8.4061D-02, &
1.8300D-03, 7.9470D-02, 1.4456D-01, 3.5820D-02, 6.0587D-02, 1.3881D-01, 1.8127D-03, 1.2050D-03, 7.8290D-02, 6.5044D-02, &
1.2073D-03, 1.3588D-01, 1.1809D-01, 1.0812D-01, 1.4497D-01, 1.0395D-01, 8.9185D-02, 7.9498D-02, 1.2183D-01, 7.5464D-02, &
1.0030D-01, 4.6630D-02, 1.2685D-01, 1.2771D-01, 7.9732D-02, 8.4769D-02, 7.4398D-02, 8.5217D-02, 5.5809D-02, 1.2458D-01, &
7.4398D-02, 7.5843D-02, 9.9442D-02, 1.2620D-01, 7.5643D-02, 9.2956D-02/), &
! Distribution coefficient, Kd(mL/g)----input from excel---need update
(/1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,              &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &

! YMF unsaturated zone data
TYPE(SITEDATA_UNSAT)::YMF_U=SITEDATA_UNSAT( &                                                    ! Unsaturated zone data for YMF site
! Volumetric water content in unsaturated zone (m^3 water/m^3 soil) Fig 7-14
0.1D0,          &
! porosity                              !(0.1-0.3) Refwork 283 p F7-11 Fig 7-10
0.2D0,          &
! Percolation rate at the unsaturated zone disposal site  (m/y))----input from excel---need update
7.5D-2,         &
! Bulk density (g/cm^3)          Refwork 283 T7-10
2.39D0,         &
! Depth form WP to the acquifer (m)  need update
6.D2,           &
! Width of the disposal site (m)                   need update
2.3269D3,       &
! Length of the disposal site (m)                  need update
2.3269D3,       &
! Depth of the disposal site (m)                   need update
1.5D2,          &
! List of element considered
(/'Ac','Ag','Am','Ba','Bi','Bk','C','Cd','Ce','Cf', &
'Cl','Cm','Co','Cs','Eu','Fe','H','He','Ho','I',       &
'Kr','Mn','Mo','Nb','Ni','Np','Pa','Pb','Pd','Pm', &
'Pu','Ra','Rh','Ru','Sb','Se','Sm','Sn','Sr','Tc',    &
'Te','Th','U','V','Y','Zr' /),         &
! Molecular diffusion coefficient (cm^2/s) EPA calculation method for diffusion coefficient-use water temp at 70 F--RefWork ID 249 + data from two websites see excel
(/7.3896D-02, 1.1733D-01, 8.4993D-02, 5.3405D-02, 7.6262D-02, 8.8141D-02, 1.7308D-01, 1.0222D-01, 7.7161D-02, 8.8427D-02,  &
1.9250D-03, 8.3597D-02, 1.5207D-01, 3.7680D-02, 6.3734D-02, 1.4602D-01, 1.9069D-03, 1.2676D-03, 8.2356D-02, 6.8422D-02,  &
1.2700D-03, 1.4293D-01, 1.2422D-01, 1.1373D-01, 1.5250D-01, 1.0935D-01, 9.3817D-02, 8.3627D-02, 1.2816D-01, 7.9383D-02,  &
1.0551D-01, 4.9052D-02, 1.3343D-01, 1.3434D-01, 8.3873D-02, 8.9172D-02, 7.8262D-02, 8.9643D-02, 5.8708D-02, 1.3105D-01,  &
7.8262D-02, 7.9783D-02, 1.0461D-01, 1.3276D-01, 7.9571D-02, 9.7784D-02/), &
! Distribution coefficient,kd(mL/g)    ----input from excel-- RefWork ID 280
(/1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,              &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,                &
1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5/))1.D-5,1.D-5,1.D-5,1.D-5,1.D-5,1.D-5/))
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Appendix F Radionuclides considered in IWMS modeling and inventories

Table F-1 Fission products and activation product in fuel meat

Nuclide name	Nuc_T12 (Years)	Nuc_ name	Nuc_At num	Nuc_A tmass	M-state	Nuc_activ (Ci)	Nuc_mass (kg)	Nuc_Heat (W)	Nuc_ATox (m^3)	Nuc_WTox (m^3)	DCF-Ing(Sv/Bq)
Ac227	2.18E+01	Ac	89	227	s	1.51E-05	2.09E-10	7.32E-09	4.99E+09	9.01E+02	3.80E-06
Ag108m	4.38E+02	Ag	47	108	m	5.60E-06	2.15E-10	5.43E-08	1.24E+05	6.96E-01	2.06E-09
Am239	1.36E-03	Am	95	239	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.67E-10
Am240	5.80E-03	Am	95	240	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.83E-10
Am241	4.33E+02	Am	95	241	s	1.20E+03	3.51E-01	4.01E+01	6.91E+16	1.30E+10	9.84E-07
Am242	1.41E+02	Am	95	242	s	2.33E+00	2.88E-09	2.69E-03	2.80E+10	3.78E+04	3.81E-10
Am242m	1.83E-03	Am	95	242	m	2.34E+00	2.24E-04	9.47E-04	1.29E+14	2.41E+07	2.10E-11
Am243	7.37E+03	Am	95	243	s	1.08E+00	5.43E-03	3.49E-02	6.23E+13	1.17E+07	9.79E-07
Am244	1.15E-03	Am	95	244	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.38E-10
Am244m	4.94E-05	Am	95	244	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.10E-11
Am245	2.34E-04	Am	95	245	s	1.74E-24	2.79E-34	3.30E-27	5.85E-17	5.85E-21	4.88E-11
Am246	4.75E-05	Am	95	246	s	1.29E-17	6.57E-28	1.05E-19	5.32E-10	4.04E-14	4.54E-11
Ba133	1.05E+01	Ba	56	133	s	1.81E-04	7.08E-10	4.88E-07	1.08E+06	1.47E+01	9.19E-10
Ba140	3.49E-02	Ba	56	140	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.56E-09
Ba141	3.47E-05	Ba	56	141	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.65E-11
Bi209	1.90E+19	Bi	83	209	s	0.00E+00	5.41E-13	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Bk249	9.03E-01	Bk	97	249	s	1.20E-19	7.33E-26	2.35E-23	1.16E-08	6.30E-15	3.24E-09
C14	5.70E+03	C	6	14	s	4.54E-03	1.02E-06	1.33E-06	1.58E+07	1.42E+02	5.64E-10
Cd113m	7.70E+15	Cd	48	113	m	5.31E-02	2.37E-07	5.78E-05	3.49E+09	6.61E+04	4.35E-08
Ce144	7.90E-02	Ce	58	144	s	1.40E-08	4.41E-15	9.19E-12	4.46E+02	3.95E-03	5.68E-09
Cf249	3.51E+02	Cf	98	249	s	3.46E-10	8.44E-14	1.29E-11	1.45E+04	6.54E-03	1.28E-06
Cf250	1.31E+01	Cf	98	250	s	1.83E-10	1.67E-15	6.80E-12	3.73E+03	1.58E-03	5.76E-07
Cf251	8.98E+02	Cf	98	251	s	5.35E-12	3.37E-15	1.92E-13	2.28E+02	1.04E-04	1.31E-06
Cf252	2.65E+00	Cf	98	252	s	3.65E-14	6.79E-20	2.64E-15	4.37E-01	1.77E-07	2.93E-07
Cl36	3.01E+05	Cl	17	36	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-10
Cm241	8.98E-02	Cm	96	241	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.21E-09
Cm242	4.46E-01	Cm	96	242	s	1.93E+00	5.83E-07	7.04E-02	6.82E+12	1.25E+06	3.10E-08
Cm243	2.91E+01	Cm	96	243	s	4.13E-01	8.00E-06	1.51E-02	1.71E+13	3.36E+06	6.79E-07
Cm244	1.81E+01	Cm	96	244	s	1.15E+01	1.41E-04	4.00E-01	3.92E+14	7.43E+07	5.45E-07
Cm245	8.50E+03	Cm	96	245	s	1.50E-03	8.73E-06	4.99E-05	8.93E+10	1.70E+04	1.01E-06
Cm246	4.76E+03	Cm	96	246	s	8.37E-05	2.72E-07	2.74E-06	4.92E+09	9.50E+02	1.00E-06
Cm247	1.56E+07	Cm	96	247	s	8.46E-11	9.35E-10	2.69E-12	4.57E+03	8.69E-04	9.24E-07
Cm248	3.48E+05	Cm	96	248	s	7.98E-11	1.88E-11	1.01E-11	1.72E+04	3.32E-03	3.68E-06
Cm249	1.23E-04	Cm	96	249	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.70E-11
Cm250	5.75E+05	Cm	96	250	s	5.15E-17	6.27E-19	3.77E-17	6.49E-02	1.23E-08	2.10E-05
Cm251	3.19E-05	Cm	96	251	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.70E-11
Cs134	2.07E+00	Cs	55	134	s	1.89E-01	1.46E-07	1.92E-03	2.26E+09	1.94E+05	1.98E-08
Cs134m	3.32E-04	Cs	55	134	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-11
Cs135	2.30E+06	Cs	55	135	s	2.59E-01	2.25E-01	8.63E-05	1.33E+09	2.80E+04	1.91E-09
Cs136	3.60E-02	Cs	55	136	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.04E-09
Cs137	3.01E+01	Cs	55	137	s	1.84E+04	2.11E-01	2.04E+01	4.30E+14	1.29E+10	1.35E-08
Cs140	2.02E-06	Cs	55	140	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-11
Cs141	7.87E-07	Cs	55	141	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-11
Cs142	5.34E-08	Cs	55	142	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-11
Cs143	5.68E-08	Cs	55	143	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-11
Cs144	3.20E-08	Cs	55	144	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-11
Cs145	1.88E-08	Cs	55	145	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-11
Cs147	7.45E-09	Cs	55	147	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-11
Eu149	2.55E-01	Eu	63	149	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.24E-10
Eu152	1.06E-03	Eu	63	152	s	1.23E+00	6.95E-06	9.37E-03	3.09E+10	9.30E+04	1.75E-09
Eu154	8.75E-05	Eu	63	154	s	6.43E+01	2.38E-04	5.84E-01	2.04E+12	6.95E+06	2.58E-09
Eu155	4.75E+00	Eu	63	155	s	3.82E+00	7.75E-06	2.97E-03	1.58E+10	6.61E+04	4.13E-10
Eu156	4.16E-02	Eu	63	156	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.48E-09
H3	1.23E+01	H	1	3	s	2.72E+01	2.81E-06	9.18E-04	4.24E+09	6.18E+04	1.73E-11
He4	3.17E+01	He	2	4	s	0.00E+00	4.45E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ho166m	1.20E+03	Ho	67	166	m	2.11E-05	1.18E-08	2.22E-07	1.52E+06	2.28E+00	2.18E-09
I129	1.57E+07	I	53	129	s	9.73E-03	5.51E-02	4.55E-06	5.59E+08	5.79E+04	7.46E-08
Kr85	5.11E-04	Kr	36	85	s	4.38E+02	1.12E-03	6.57E-01	2.46E+08	4.38E+02	0.00E+00
Mo93	4.00E+03	Mo	42	93	s	1.55E-09	1.41E-12	1.47E-13	2.14E+00	2.60E-04	3.64E-10
Nb91	1.67E-01	Nb	41	91	s	5.11E-09	8.84E-13	5.19E-13	5.11E-09	5.11E-09	0.00E+00
Nb93m	1.61E+01	Nb	41	93	m	5.92E-01	2.48E-06	1.02E-04	6.40E+08	3.85E+03	1.41E-10
Nb94	2.03E+04	Nb	41	94	s	3.63E-05	1.94E-07	3.69E-07	1.07E+06	3.33E+00	1.93E-09
Nb95	9.88E-03	Nb	41	95	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.95E-10
Nb95m	9.58E-02	Nb	41	95	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.22E-10
Ni59	7.60E+04	Ni	28	59	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.67E-11

Nuclide name	Nuc_T12 (Years)	Nuc_ name	Nuc_At num	Nuc_A tmass	M-state	Nuc_activ (Ci)	Nuc_mass (kg)	Nuc_Heat (W)	Nuc_ATox (m^3)	Nuc_WTox (m^3)	DCF-Ing(Sv/Bq)
Ni63	1.00E+02	Ni	28	63	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.56E-10
Np235	1.08E+00	Np	93	235	s	2.84E-13	2.03E-19	1.68E-17	1.07E-04	8.15E-10	6.56E-11
Np236	1.53E+05	Np	93	236	s	4.02E-07	3.05E-08	8.21E-10	1.93E+06	3.68E-01	2.34E-07
Np236m	2.57E-03	Np	93	236	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.70E-10
Np237	2.14E+06	Np	93	237	s	9.49E-02	1.35E-01	2.71E-03	2.85E+12	5.65E+05	1.20E-06
Np238	5.80E-03	Np	93	238	s	1.05E-02	4.07E-11	5.26E-05	2.22E+07	5.19E+02	1.08E-09
Np239	6.45E-03	Np	93	239	s	1.08E+00	4.67E-09	2.74E-03	6.49E+08	4.69E+04	8.82E-10
Np240	1.37E-05	Np	93	240	s	5.29E-12	4.18E-22	5.08E-14	2.86E-04	2.34E-08	6.40E-11
Np240m	1.37E-05	Np	93	240	m	4.41E-09	4.06E-20	2.47E-11	4.41E-09	4.41E-09	0.00E+00
Np241	2.64E-05	Np	93	241	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pa231	3.28E+04	Pa	91	231	s	3.17E-05	6.71E-07	9.65E-07	2.66E+09	1.22E+03	2.86E-06
Pb206	3.96E-12	Pb	82	206	s	0.00E+00	3.87E-12	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pb207	2.55E-08	Pb	82	207	s	0.00E+00	9.77E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pb208	3.17E+01	Pb	82	208	s	0.00E+00	2.83E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pb210	2.22E+01	Pb	82	210	s	9.86E-07	1.29E-11	2.31E-10	3.31E+06	3.68E+01	1.45E-06
Pd107	6.50E+06	Pd	46	107	s	3.08E-02	5.98E-02	1.70E-06	1.09E+07	6.16E+01	4.04E-11
Pm146	5.53E+00	Pm	61	146	s	1.78E-03	4.02E-09	8.88E-06	2.24E+07	8.64E+01	9.91E+10
Pm147	2.62E+00	Pm	61	147	s	9.01E+00	9.72E-06	3.31E-03	2.71E+10	1.27E+05	2.83E-10
Pu236	2.86E+00	Pu	94	236	s	7.42E-06	1.42E-11	2.58E-07	1.78E+08	3.48E+01	3.15E-07
Pu237	1.24E-01	Pu	94	237	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E-10
Pu238	8.77E+01	Pu	94	238	s	2.61E+02	1.52E-02	8.65E+00	1.72E+16	3.25E+09	8.65E-07
Pu239	2.41E+04	Pu	94	239	s	2.51E+02	4.04E+00	7.80E+00	1.81E+16	3.39E+09	9.56E-07
Pu240	6.56E+03	Pu	94	240	s	2.18E+02	9.59E-01	6.78E+00	1.57E+16	2.94E+09	9.56E-07
Pu241	1.43E+01	Pu	94	241	s	8.13E+03	7.86E-02	2.58E-01	1.12E+16	2.11E+09	1.85E-08
Pu242	3.74E+05	Pu	94	242	s	2.55E-01	6.44E-02	7.52E-03	1.68E+13	3.30E+06	9.08E-07
Pu243	5.65E-04	Pu	94	243	s	8.46E-11	3.25E-20	9.74E-14	4.36E-03	3.88E-07	9.02E-11
Pu244	7.99E+07	Pu	94	244	s	4.41E-09	2.41E-07	1.28E-10	2.90E+05	5.72E-02	8.97E-07
Pu246	2.97E-02	Pu	94	246	s	1.29E-17	2.63E-25	1.95E-20	6.19E-08	2.30E-12	3.66E-09
Ra226	1.60E+03	Ra	88	226	s	3.29E-06	3.33E-09	9.51E-08	1.88E+07	4.98E+01	3.58E-07
Ra228	5.75E+00	Ra	88	228	s	1.92E-10	7.02E-16	1.06E-14	1.84E+03	7.15E-03	3.88E-07
Rh102	3.74E+00	Rh	45	102	s	2.56E-11	4.14E-18	1.01E-13	2.61E-01	3.60E-06	2.82E-09
Ru106	1.02E+00	Ru	44	106	s	6.48E-06	1.95E-12	3.85E-10	2.56E+05	2.45E+00	7.40E-09
Sb124	1.65E-01	Sb	51	124	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.74E-09
Sb124m	2.95E-06	Sb	51	124	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.91E-12
Sb125	2.76E+00	Sb	51	125	s	3.89E-01	3.71E-07	1.23E-03	2.80E+09	2.32E+04	7.59E-10
Sb126	3.38E-02	Sb	51	126	s	2.49E-02	2.98E-10	4.60E-04	4.78E+07	3.23E+03	2.89E-09
Se79	2.95E+05	Se	34	79	s	2.96E-02	1.93E-03	9.80E-06	1.21E+08	4.65E+03	2.35E-09
Sm145	9.31E-01	Sm	62	145	s	3.34E-15	1.26E-21	1.83E-18	3.21E-06	3.79E-11	2.46E-10
Sm146	1.03E+08	Sm	62	146	s	2.59E-08	1.09E-06	3.90E-10	1.70E+05	7.54E-02	5.51E-08
Sm148	7.00E+15	Sm	62	148	s	8.93E-12	2.93E-02	1.05E-13	8.93E-12	8.93E-12	0.00E+00
Sm151	9.00E+01	Sm	62	151	s	1.83E+02	6.95E-03	2.15E-02	4.39E+11	9.68E+05	1.05E-10
Sm155	4.24E-05	Sm	62	155	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.93E-11
Sn117m	3.72E-02	Sn	50	117	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.97E-10
Sn119m	8.02E-01	Sn	50	119	m	9.53E-13	2.54E-19	4.93E-16	1.26E-03	1.75E-08	3.76E-10
Sn121m	5.50E+01	Sn	50	121	m	2.86E+00	5.31E-05	6.60E-04	7.72E+09	5.86E+04	4.19E-10
Sn123	3.54E-01	Sn	50	123	s	7.28E-28	8.85E-35	2.27E-30	3.53E-18	8.26E-23	2.27E-09
Sn125	2.64E-02	Sn	50	125	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.33E-09
Sn125m	1.81E-05	Sn	50	125	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sn126	2.30E+05	Sn	50	126	s	1.78E-01	6.26E-03	2.77E-04	2.99E+09	4.51E+04	5.27E-09
Sr103	2.19E-09	Sr	38	103	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sr87m	3.21E-04	Sr	38	87	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.58E-11
Sr89	1.38E-01	Sr	38	89	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.50E-09
Sr90	2.88E+01	Sr	38	90	s	1.39E+04	9.86E-02	1.62E+01	1.34E+15	2.11E+10	3.85E-08
Sr91	1.10E-03	Sr	38	91	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.39E-10
Sr93	1.41E-05	Sr	38	93	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sr95	7.57E-07	Sr	38	95	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sr99	8.56E-09	Sr	38	99	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Tc98	4.20E+06	Tc	43	98	s	7.62E-07	8.77E-07	6.85E-09	2.06E+04	8.24E-02	1.32E-09
Tc99	6.86E-04	Tc	43	99	s	5.68E+00	3.32E-01	2.85E-03	4.44E+10	1.96E+05	3.95E-10
Te125m	1.57E-01	Te	52	125	m	9.50E-02	5.27E-09	8.00E-05	2.39E+08	4.46E+03	9.92E-10
Th228	1.91E+00	Th	90	228	s	1.97E-03	2.40E-09	6.44E-05	4.71E+10	7.65E+03	1.07E-07
Th229	7.34E+03	Th	90	229	s	6.57E-08	3.31E-10	2.02E-09	9.45E+06	1.74E+00	9.54E-04
Th230	7.54E+04	Th	90	230	s	4.05E-04	1.96E-05	1.14E-05	2.42E+10	4.59E+03	1.48E-07
Th232	1.41E+10	Th	90	232	s	2.47E-10	2.25E-06	5.97E-12	1.62E+04	3.07E-03	7.38E-07
U232	6.89E+01	U	92	232	s	1.91E-03	8.66E-08	6.13E-05	4.24E+10	3.41E+04	3.54E-07
U233	1.59E+05	U	92	233	s	2.32E-05	2.40E-06	6.75E-07	1.33E+08	6.38E+01	7.81E-08
U234	2.45E+05	U	92	234	s	1.18E+00	1.89E-01	3.38E-02	6.64E+12	3.11E+06	7.66E-08
U235	7.04E+08	U	92	235	s	3.07E-02	1.42E+01	8.51E-04	1.57E+11	7.80E+04	7.19E-08
U236	2.34E+07	U	92	236	s	1.36E-01	2.11E+00	3.69E-03	7.10E+11	3.46E+05	7.26E-08
U237	1.85E-02	U	92	237	s	1.95E-01	2.38E-09	3.77E-04	2.22E+08	8.00E+03	8.48E-10
U238	4.47E+09	U	92	238	s	3.24E-01	9.65E+02	8.21E-03	1.56E+12	7.89E+05	6.88E-08
Y91	1.60E-01	Y	39	91	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.57E-09
Y93	1.16E-03	Y	39	93	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.23E-09
Zr93	1.53E+06	Zr	40	93	s	7.48E-01	2.98E-01	8.42E-05	1.12E+10	4.45E+04	4.48E-09
Zr95	1.75E-01	Zr	40	95	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E-09
Ot260	3.17E-04	Ot	99	260	s	6.73E+00	1.01E+01	0.00E+00	4.92E+13	4.88E+06	0.00E+00

Table F-2 Fission products and activation product in fuel clad

Nuclide name	Nuc_T12 (Years)	Nuc_ name	Nuc_At num	Nuc_At mass	M-state	Nuc_activ (Ci)	Nuc_mass (kg)	Nuc_Heat (W)	Nuc_ATox (m^3)	Nuc_WTox (m^3)	DCF-Ing(Sv/Bq)
C14	5.70E+03	C	6	14	s	5.87E-02	1.32E-05	1.72E-05	2.04E+08	1.84E+03	5.64E-10
Cd109	1.26E+00	Cd	48	109	s	7.22E-11	2.79E-17	8.44E-15	3.51E-01	7.81E-06	3.55E-09
Cd113m	7.69E+15	Cd	48	113	m	2.48E-09	1.11E-14	2.70E-12	1.63E+02	3.09E-03	4.35E-08
Co58	1.94E-01	Co	27	58	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.68E-10
Co60	5.27E+00	Co	27	60	s	1.24E+00	1.10E-06	1.91E-02	2.30E+10	2.28E+05	7.28E-09
Fe55	2.74E+00	Fe	26	55	s	1.37E-02	5.74E-09	4.65E-07	6.33E+06	2.44E+02	1.64E-10
H3	1.23E+01	H	1	3	s	1.85E-07	1.91E-14	6.23E-12	2.88E+01	4.20E-04	1.73E-11
Mn54	8.55E-01	Mn	25	54	s	8.94E-12	1.15E-18	4.45E-14	8.05E-03	3.43E-07	7.48E-10
Nb91	6.80E+02	Nb	41	91	s	5.51E-06	9.54E-10	5.60E-10	5.51E-06	5.51E-06	0.00E+00
Nb92	3.47E+07	Nb	41	92	s	2.96E-07	2.67E-06	2.66E-09	2.96E-07	2.96E-07	0.00E+00
Nb93m	1.61E+01	Nb	41	93	m	4.57E+00	1.92E-05	7.85E-04	4.94E+09	2.97E+04	1.41E-10
Nb94	2.03E+04	Nb	41	94	s	5.26E-01	2.80E-03	5.35E-03	1.55E+10	4.82E+04	1.93E-09
Nb95	9.58E-02	Nb	41	95	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.95E-10
Ni59	7.59E+04	Ni	28	59	s	9.63E-04	1.19E-05	4.20E-08	4.79E+05	3.28E+00	5.67E-11
Ni63	1.00E+02	Ni	28	63	s	9.34E-02	1.65E-06	9.49E-06	1.12E+08	7.59E+02	1.56E-10
Sb125	2.76E+00	Sb	51	125	s	4.77E-02	4.55E-08	1.51E-04	3.43E+08	2.84E+03	7.59E-10
Sn119m	8.02E-01	Sn	50	119	m	2.72E-10	7.26E-17	1.41E-13	3.59E-01	5.00E-06	3.76E-10
Sn121	3.08E-03	Sn	50	121	s	1.27E-01	1.33E-10	8.67E-05	1.75E+07	1.58E+03	2.44E-10
Sn121m	4.39E+01	Sn	50	121	m	1.64E-01	3.04E-06	3.78E-05	4.42E+08	3.36E+03	4.19E-10
Sr90	2.89E+01	Sr	38	90	s	8.70E-05	6.17E-10	1.01E-07	8.37E+06	1.32E+02	3.85E-08
Tc99	2.11E+05	Tc	43	99	s	5.47E-07	3.20E-08	2.74E-10	4.27E+03	1.89E-02	3.95E-10
Te125m	1.57E-01	Te	52	125	m	1.17E-02	6.46E-10	9.80E-06	2.93E+07	5.47E+02	9.92E-10
V49	9.03E-01	V	23	49	s	7.29E-18	9.24E-25	1.91E-22	1.49E-10	7.08E-15	1.66E-11
Y90	7.31E-03	Y	39	90	s	8.71E-05	1.60E-13	4.82E-07	7.84E+04	1.27E+01	2.91E-09
Zr93	1.53E+06	Zr	40	93	s	4.22E-02	1.68E-02	4.75E-06	6.32E+08	2.51E+03	4.48E-10
Ot261	3.17E-04	Ot	99	261	s	8.46E-04	3.62E+02	0.00E+00	1.59E+06	2.75E+01	0.00E+00

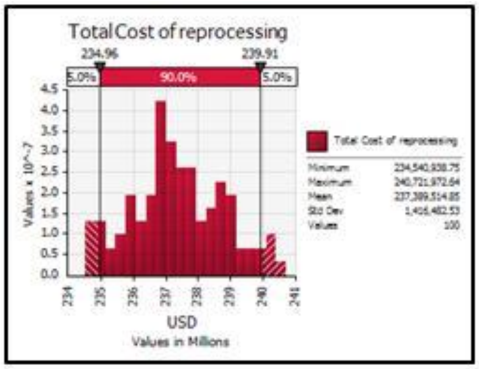
Table F-3 Fission products and activation product in structure materials

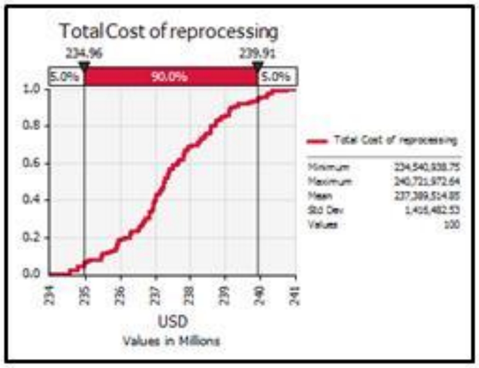
Nuclide name	Nuc_T12 (Years)	Nuc_ name	Nuc_At num	Nuc_At mass	M-state	Nuc_activ (Ci)	Nuc_mass (kg)	Nuc_Heat (W)	Nuc_ATox (m^3)	Nuc_WTox (m^3)	DCF-Ing(Sv/Bq)
C14	5.696E+03	C	6	14	s	5.87E-02	1.32E-05	1.72E-05	2.04E+08	1.84E+03	5.64E-10
Co58	1.940E-01	Co	27	58	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.68E-10
Co60	5.271E+00	Co	27	60	s	3.99E+01	3.53E-05	6.15E-01	7.42E+11	7.33E+06	7.28E-09
Fe55	7.493E-03	Fe	26	55	s	3.68E-01	1.55E-07	1.25E-05	1.70E+08	6.56E+03	1.64E-10
Fe59	5.076E-03	Fe	26	59	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.81E-09
Mn54	2.408E-03	Mn	25	54	s	2.19E-10	2.82E-17	1.09E-12	1.97E-01	8.37E-06	7.48E-10
Nb93m	1.61E+01	Nb	41	93	m	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.41E-10
Nb94	2.03E+04	Nb	41	94	s	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.93E-09
Ni59	7.595E+04	Ni	28	59	s	2.10E+00	2.60E-02	9.16E-05	1.05E+09	7.14E+03	5.67E-11
Ni63	1.000E+02	Ni	28	63	s	2.04E+02	3.59E-03	2.07E-02	2.44E+11	1.66E+06	1.56E-10
Ot262	3.17E-04	Ot	99	262	s	2.47E-02	1.64E+02	7.15E-05	0.00E+00	0.00E+00	0.00E+00

Appendix G Probabilistic results of IWMS global outputs

@RISK Output Report for Total Cost of reprocessing

Performed By: bsrimok
Date: Thursday, June 30, 2011 12:00:31 AM





Simulation Summary Information

Workbook Name	IWMS.xlsm
Number of Simulations	1
Number of Iterations	100
Number of Inputs	241
Number of Outputs	9
Sampling Type	Latin Hypercube
Simulation Start Time	6/29/11 14:53:22
Simulation Duration	09:07:05
Random # Generator	Mersenne Twister
Random Seed	1319015524

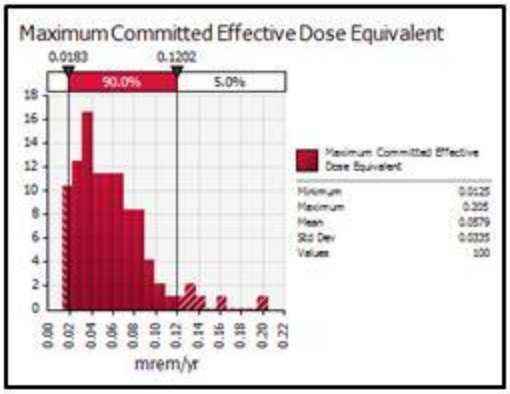
Summary Statistics for Total Cost of reprocessing

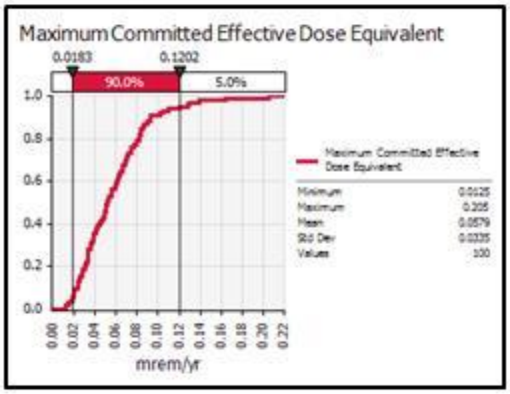
Statistics		Percentile	
Minimum	2.345409E+08	**5%**	2.349641E+08
Maximum	2.407220E+08	**10%**	2.354678E+08
Mean	2.373895E+08	**15%**	2.358817E+08
Std Dev	1.416483E+06	**20%**	2.361377E+08
Variance	2.00642E+12	**25%**	2.365394E+08
Skewness	0.131378034	**30%**	2.367272E+08
Kurtosis	2.610203517	**35%**	2.369152E+08
Median	2.372522E+08	**40%**	2.369750E+08
Mode	2.368281E+08	**45%**	2.371106E+08
Left X	2.349641E+08	**50%**	2.372522E+08
Left P	5%	**55%**	2.373877E+08
Right X	2.399071E+08	**60%**	2.376041E+08
Right P	95%	**65%**	2.377973E+08
Diff X	4.943002E+06	**70%**	2.380363E+08
Diff P	90%	**75%**	2.384117E+08
#Errors	0	**80%**	2.385931E+08
Filter Min	Off	**85%**	2.388774E+08
Filter Max	Off	**90%**	2.391400E+08
#Filtered	0	**95%**	2.399071E+08

@RISK Output Report for Maximum Committed Effective Dose Equivalent

Performed By: bsrimok

Date: Thursday, June 30, 2011 12:00:31 AM





Simulation Summary Information

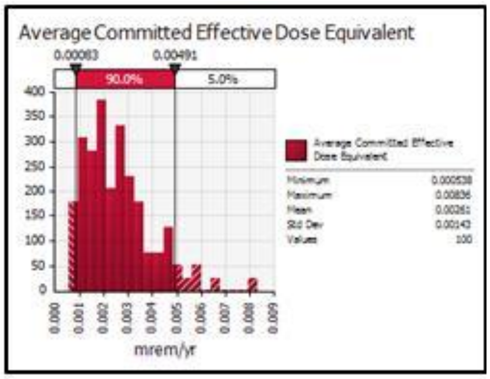
Workbook Name	IWMS.xlsm
Number of Simulations	1
Number of Iterations	100
Number of Inputs	241
Number of Outputs	9
Sampling Type	Latin Hypercube
Simulation Start Time	6/29/11 14:53:22
Simulation Duration	09:07:05
Random # Generator	Mersenne Twister
Random Seed	1319015524

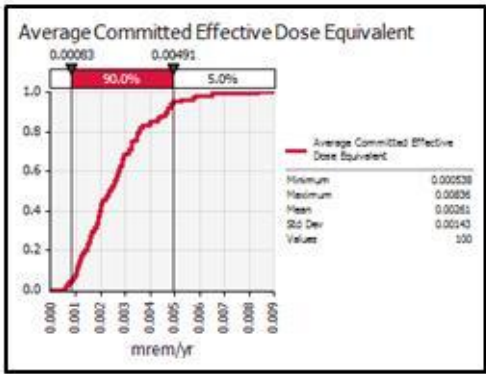
Summary Statistics for Maximum Committed Effective Dose Equivalent

Statistics		**Percentile**	
Minimum	1.251650E-02	**5%**	1.831939E-02
Maximum	2.051201E-01	**10%**	2.081047E-02
Mean	5.785123E-02	**15%**	2.547159E-02
Std Dev	3.345387E-02	**20%**	3.037953E-02
Variance	0.001119162	**25%**	3.308579E-02
Skewness	1.489035265	**30%**	3.639099E-02
Kurtosis	6.589558254	**35%**	3.836189E-02
Median	5.128609E-02	**40%**	4.397513E-02
Mode	2.015422E-02	**45%**	4.858950E-02
Left X	1.831939E-02	**50%**	5.128609E-02
Left P	5%	**55%**	5.568660E-02
Right X	1.201844E-01	**60%**	6.031194E-02
Right P	95%	**65%**	6.432935E-02
Diff X	1.018650E-01	**70%**	6.910452E-02
Diff P	90%	**75%**	7.455361E-02
#Errors	0	**80%**	8.214558E-02
Filter Min	Off	**85%**	8.480496E-02
Filter Max	Off	**90%**	9.292599E-02
#Filtered	0	**95%**	1.201844E-01

@RISK Output Report for Average Committed Effective Dose Equivalent

Performed By: bsrimok
Date: Thursday, June 30, 2011
12:00:31 AM





Simulation Summary Information

Workbook Name	IWMS.xlsm
Number of Simulations	1
Number of Iterations	100
Number of Inputs	241
Number of Outputs	9
Sampling Type	Latin Hypercube
Simulation Start Time	6/29/11 14:53:22
Simulation Duration	09:07:05
Random # Generator	Mersenne Twister
Random Seed	1319015524

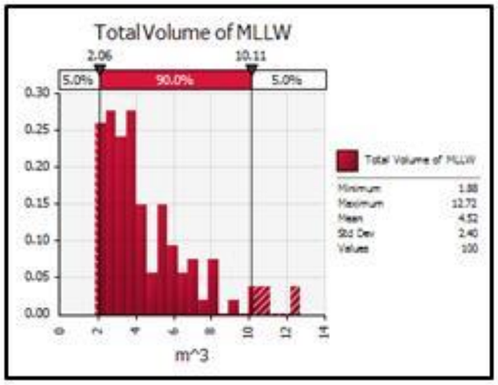
Summary Statistics for Average Committed Effective Dose Equivalent

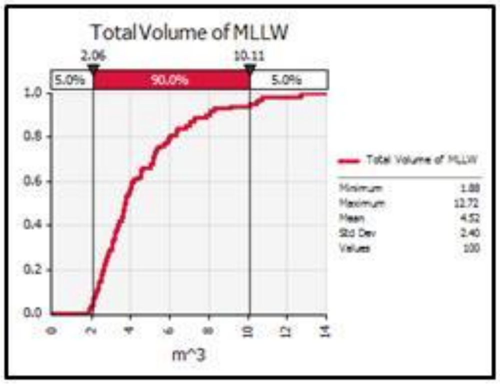
Statistics		**Percentile**	
Minimum	5.383085E-04	**5%**	8.330985E-04
Maximum	8.355803E-03	**10%**	1.034909E-03
Mean	2.607090E-03	**15%**	1.139239E-03
Std Dev	1.429787E-03	**20%**	1.340555E-03
Variance	2.04429E-06	**25%**	1.556870E-03
Skewness	1.150405799	**30%**	1.700360E-03
Kurtosis	4.895912569	**35%**	1.879192E-03
Median	2.329142E-03	**40%**	1.973099E-03
Mode	1.485277E-03	**45%**	2.067328E-03
Left X	8.330985E-04	**50%**	2.329142E-03
Left P	5%	**55%**	2.560371E-03
Right X	4.911593E-03	**60%**	2.730105E-03
Right P	95%	**65%**	2.877619E-03
Diff X	4.078495E-03	**70%**	3.141657E-03
Diff P	90%	**75%**	3.270396E-03
#Errors	0	**80%**	3.515974E-03
Filter Min	Off	**85%**	4.015873E-03
Filter Max	Off	**90%**	4.644783E-03
#Filtered	0	**95%**	4.911593E-03

@RISK Output Report for Total Volume of MLLW

Performed By: bsrimok

Date: Thursday, June 30, 2011 12:00:30 AM





Simulation Summary Information

Workbook Name	IWMS.xlsm
Number of Simulations	1
Number of Iterations	100
Number of Inputs	241
Number of Outputs	9
Sampling Type	Latin Hypercube
Simulation Start Time	6/29/11 14:53:22
Simulation Duration	09:07:05
Random # Generator	Mersenne Twister
Random Seed	1319015524

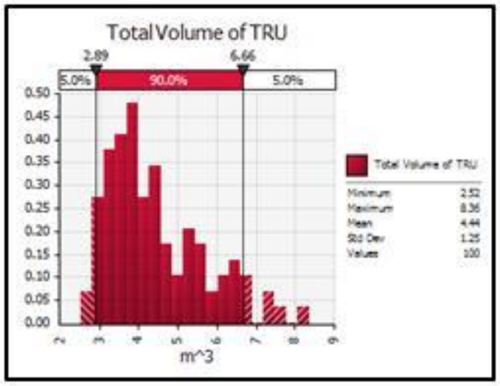
Summary Statistics for Total Volume of MLLW

Statistics		**Percentile**	
Minimum	1.883200E+00	**5%**	2.060970E+00
Maximum	1.272142E+01	**10%**	2.218832E+00
Mean	4.521994E+00	**15%**	2.467091E+00
Std Dev	2.398698E+00	**20%**	2.591090E+00
Variance	5.753750662	**25%**	2.784996E+00
Skewness	1.510260573	**30%**	3.036638E+00
Kurtosis	5.13373466	**35%**	3.227541E+00
Median	3.713468E+00	**40%**	3.362962E+00
Mode	4.068696E+00	**45%**	3.601671E+00
Left X	2.060970E+00	**50%**	3.713468E+00
Left P	5%	**55%**	3.905213E+00
Right X	1.010651E+01	**60%**	4.076807E+00
Right P	95%	**65%**	4.552715E+00
Diff X	8.045541E+00	**70%**	5.171840E+00
Diff P	90%	**75%**	5.360051E+00
#Errors	0	**80%**	6.024839E+00
Filter Min	Off	**85%**	6.816740E+00
Filter Max	Off	**90%**	7.885728E+00
#Filtered	0	**95%**	1.010651E+01

@RISK Output Report for Total Volume of TRU

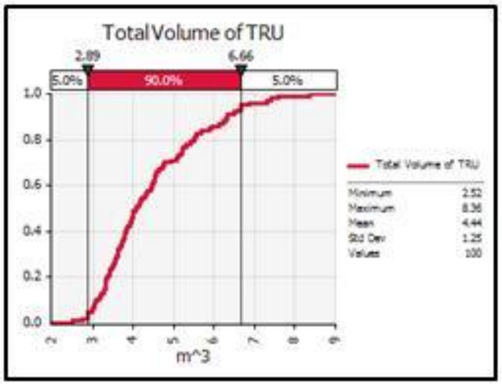
Performed By: bsrimok

Date: Thursday, June 30, 2011 12:00:30 AM



Simulation Summary Information

Workbook Name	IWMS.xlsm
Number of Simulations	1
Number of Iterations	100
Number of Inputs	241
Number of Outputs	9
Sampling Type	Latin Hypercube
Simulation Start Time	6/29/11 14:53:22
Simulation Duration	09:07:05
Random # Generator	Mersenne Twister
Random Seed	1319015524



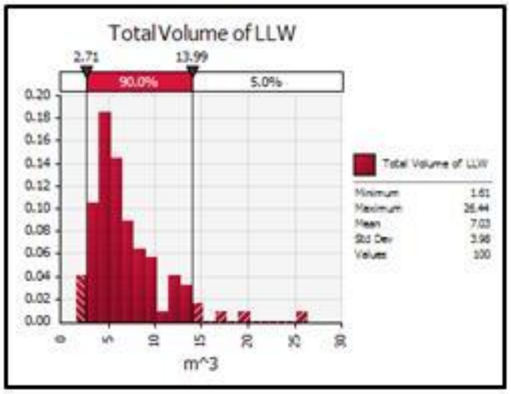
Summary Statistics for Total Volume of TRU

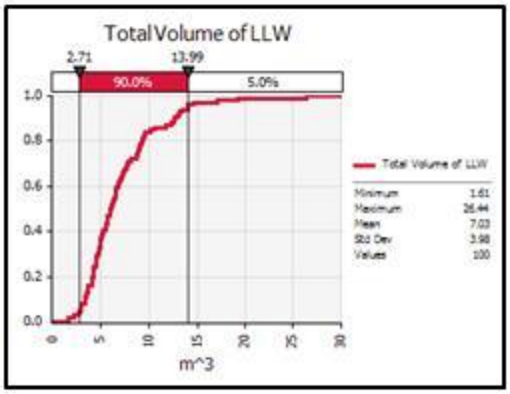
Statistics		**Percentile**	
Minimum	2.523219E+00	**5%**	2.890182E+00
Maximum	8.357906E+00	**10%**	3.067080E+00
Mean	4.437781E+00	**15%**	3.277479E+00
Std Dev	1.248811E+00	**20%**	3.347381E+00
Variance	1.55952895	**25%**	3.487202E+00
Skewness	0.944544881	**30%**	3.617123E+00
Kurtosis	3.310659805	**35%**	3.709278E+00
Median	4.055362E+00	**40%**	3.819145E+00
Mode	3.310666E+00	**45%**	3.948145E+00
Left X	2.890182E+00	**50%**	4.055362E+00
Left P	5%	**55%**	4.219677E+00
Right X	6.655595E+00	**60%**	4.457007E+00
Right P	95%	**65%**	4.557254E+00
Diff X	3.765413E+00	**70%**	4.780668E+00
Diff P	90%	**75%**	5.204328E+00
#Errors	0	**80%**	5.469243E+00
Filter Min	Off	**85%**	5.887601E+00
Filter Max	Off	**90%**	6.327985E+00
#Filtered	0	**95%**	6.655595E+00

@RISK Output Report for Total Volume of LLW

Performed By: bsrimok

Date: Thursday, June 30, 2011 12:00:30 AM





Simulation Summary Information	
Workbook Name	IWMS.xlsm
Number of Simulations	1
Number of Iterations	100
Number of Inputs	241
Number of Outputs	9
Sampling Type	Latin Hypercube
Simulation Start Time	6/29/11 14:53:22
Simulation Duration	09:07:05
Random # Generator	Mersenne Twister
Random Seed	1319015524

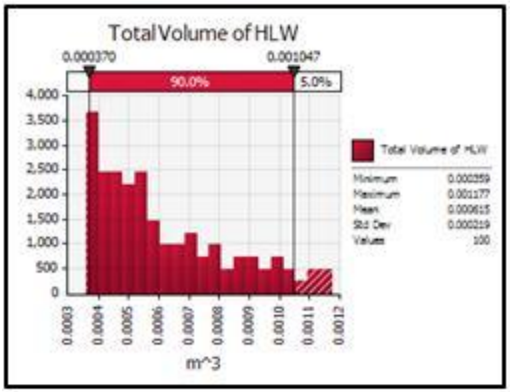
Summary Statistics for Total Volume of LLW

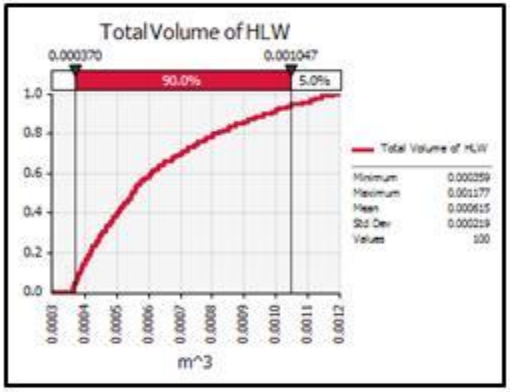
Statistics		Percentile	
Minimum	1.606442E+00	**5%**	2.714437E+00
Maximum	2.643625E+01	**10%**	3.388545E+00
Mean	7.029991E+00	**15%**	3.615639E+00
Std Dev	3.980424E+00	**20%**	4.130258E+00
Variance	15.84377888	**25%**	4.299278E+00
Skewness	1.863457468	**30%**	4.691346E+00
Kurtosis	8.379827425	**35%**	4.880018E+00
Median	5.989870E+00	**40%**	5.150299E+00
Mode	4.133244E+00	**45%**	5.654523E+00
Left X	2.714437E+00	**50%**	5.989870E+00
Left P	5%	**55%**	6.410094E+00
Right X	1.398578E+01	**60%**	6.681759E+00
Right P	95%	**65%**	7.262337E+00
Diff X	1.127134E+01	**70%**	7.713959E+00
Diff P	90%	**75%**	8.832698E+00
#Errors	0	**80%**	9.219175E+00
Filter Min	Off	**85%**	1.019272E+01
Filter Max	Off	**90%**	1.267802E+01
#Filtered	0	**95%**	1.398578E+01

@RISK Output Report for Total Volume of HLW

Performed By: bsrimok

Date: Thursday, June 30, 2011 12:00:29 AM





Simulation Summary Information

Workbook Name	IWMS.xlsm
Number of Simulations	1
Number of Iterations	100
Number of Inputs	241
Number of Outputs	9
Sampling Type	Latin Hypercube
Simulation Start Time	6/29/11 14:53:22
Simulation Duration	09:07:05
Random # Generator	Mersenne Twister
Random Seed	1319015524

Summary Statistics for Total Volume of HLW

Statistics		**Percentile**	
Minimum	3.590950E-04	**5%**	3.702970E-04
Maximum	1.176740E-03	**10%**	3.840500E-04
Mean	6.154392E-04	**15%**	3.995480E-04
Std Dev	2.192300E-04	**20%**	4.161090E-04
Variance	4.80618E-08	**25%**	4.343820E-04
Skewness	0.884599222	**30%**	4.545620E-04
Kurtosis	2.77681472	**35%**	4.780960E-04
Median	5.483600E-04	**40%**	4.989890E-04
Mode	4.150487E-04	**45%**	5.247550E-04
Left X	3.702970E-04	**50%**	5.483600E-04
Left P	5%	**55%**	5.722580E-04
Right X	1.046900E-03	**60%**	6.043830E-04
Right P	95%	**65%**	6.472910E-04
Diff X	6.766030E-04	**70%**	6.962500E-04
Diff P	90%	**75%**	7.477130E-04
#Errors	0	**80%**	8.040180E-04
Filter Min	Off	**85%**	8.727870E-04
Filter Max	Off	**90%**	9.605850E-04
#Filtered	0	**95%**	1.046900E-03