

# The FIT Model – Fuel-Cycle Integration and Tradeoffs

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**September 2010**

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## SUMMARY

All mass streams from fuel separation and fabrication are products that must meet some set of product criteria – fuel feedstock impurity limits, waste acceptance criteria (WAC), material storage (if any), or recycle material purity requirements such as zirconium for cladding or lanthanides for industrial use.<sup>a</sup> These must be considered in a systematic and comprehensive way. The FIT model and the “system losses study” team that developed it [Shropshire2009, Piet2010] are an initial step by the FCR&D program toward a global analysis that accounts for the requirements and capabilities of each component, as well as major material flows within an integrated fuel cycle. This will help the program identify near-term R&D needs and set longer-term goals.

The question originally posed to the “system losses study” was the cost of separation, fuel fabrication, waste management, etc. versus the separation efficiency. In other words, are the costs associated with marginal reductions in separations losses (or improvements in product recovery) justified by the gains in the performance of other systems? How much can be spent on remote fuel fabrication and separation without unacceptably impacting cost? Now, given what we have learned and how the FCR&D program has evolved, we ask the question: how does one adjust the compositions and quantities of all mass streams, given uncertain product criteria, to balance competing objectives including cost?

FIT is a method to analyze different fuel cycles using common bases to determine how chemical performance changes in one part of a fuel cycle (say used fuel cooling times or separation efficiencies) affect other parts of the fuel cycle. FIT estimates impurities in fuel and waste via a rough estimate of physics and mass balance for a set of technologies. If feasibility is an issue for a set, as it is for “minimum fuel treatment” approaches such as melt refining and AIROX, it can help to make an estimate of how performances would have to change to achieve feasibility.

FIT 1.0 is a “mass flow engine” (Figure S-1) that posits an incoming flow of used fuel, an initial separation with mass flows to fabrication and waste forms. Recycling flows link a second separation of used fuel to a reactor and fabrication in a loop. The feed stream blending module associated with fuel fabrication can mix TRU-U-1 and RU-1 from separation-1, TRU-U-2 and RU-2 from separation-2, and depleted uranium (RU) to keep the mixture’s k-effective approximately equally to that for a user-selected

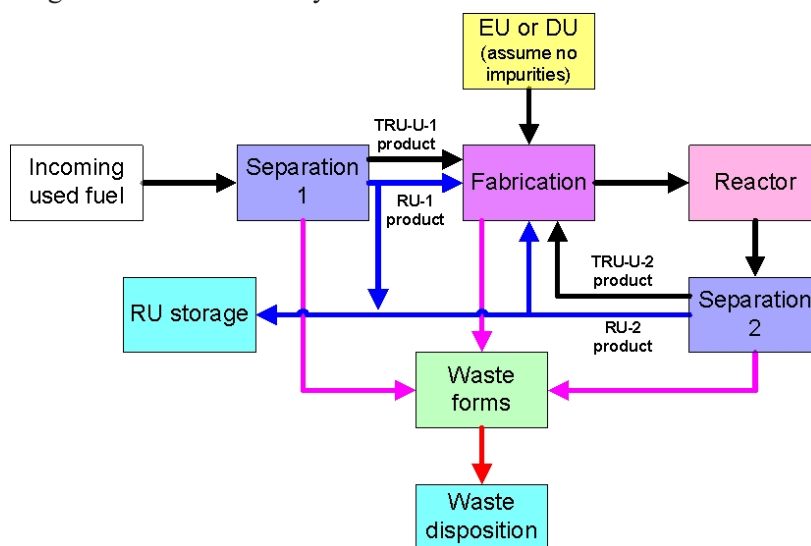


Figure S-1. Basic mass flows; the tool does not address EU feed.

<sup>a</sup> China, which mines 93% of the world’s lanthanides and has 99% of the known supply of many of them, is currently blocking such exports to Japan. See Keith Bradsher, “Amid Tension, China Blocks Vital Exports to Japan,” New York Times, September 22, 2010, [www.nytimes.com/2010/09/23/business/global/23rare.html](http://www.nytimes.com/2010/09/23/business/global/23rare.html). The lanthanides are used for solar panels, generators in wind turbines, motors in hybrid cars, “rangefinders on the Army’s tanks, sonar systems aboard Navy vessels and the control vanes on the Air Force’s smart bombs.” In nature, they are typically found with the actinides because of chemical similarity; the same reason the actinide-lanthanide separation is a challenge in used fuel separation. We note that the many lanthanide fission products have no medium or long-lived radioactive isotopes and, if pure, would be non-radioactive within a few years. And, the lanthanides as a class would appear candidates for near-surface burial.[Piet2009] Can they be economically recovered from used fuel?

impurity-free fuel recipe. The flow of TRU-U-1 is kept constant; the flow of TRU-U-2 is the residual mass from the preceding recycle. The selection among RU-1, RU-2, or DU is user controlled. Users can add or change the “static” user-defined separation matrices (x% of elements go into which product stream). FIT 1.0 was not intended to be a stand-alone tool; it is only for use by the “losses study” team.

In the current FY2011 budget, FIT 2.0 is to become more user-friendly with a physics driver (MrTauWinery) that incorporates fission products (possibly tracking individual transition metal elements), and more waste management outputs (possibly with automated waste classification, based on user-definition of waste classes). As needs arise, users could add new fuel modules.

Additional capabilities, subject to program priorities, include tracking of impurities other than fission products, options for input of enriched uranium (EU) and/or natural uranium (NU), by-passing separation-1 (as required for a breeder), thorium fuels, economics, and an “optimizer” or “solver” that would automatically iterate the mass flow engine to balance criteria or to meet a particular criteria.

Table S-1 lists FY2010 and potential future cases for FIT analysis.

Table S-1. Current and potential use cases

Lead-in Step (source of feed material for the recirculation part of system)	Recycling Loop	Comment
None	Metal/fast reactor/echem Oxide/fast reactor/UREX+1	FY 2009 analysis
UOX/UREX+1	<i>Both</i>	Complete 1-tier, <b>done in FY 2010</b>
UOX/AIROX	Metal/ fast reactor/melt refine Oxide/ fast reactor/AIROX	Minimum fuel treatment, <b>done in FY 2010</b>
UOX/UREX+1	Metal/ fast reactor/UREX+1 Oxide/ fast reactor/echem	Switch the technologies for fuel fabrication and fuel separation (metal fuel with UREX+1 and oxide fuel with echem). FIT 1.0 could analyze this case.
MOX/UREX+1	<i>Both</i>	FIT 1.0 could analyze this case.
UOX/UREX+1 With long interim storage	<i>Both</i>	FIT 1.0 could analyze this case.
UOX/UREX+1 Without CsSr removal	<i>Both</i>	FIT 1.0 could analyze this case.
UOX/NUEX	<i>Both</i>	Requires separation matrix for NUEX.
UOX/COEX	<i>Both</i>	Requires separation matrix for COEX.
Options using enriched uranium in the recycle loop		Requires adding EU as a uranium blending option
Breeder reactors in the recycle loop		Requires adding NU as a uranium blending option
Fuels other than oxide or metal in the recycle loop, e.g., TRISO fuel for HTGRs		Requires new fuel modules
Reactors other than FR in the recycle loop, e.g., CANDU		May only require appropriate physics data for that reactor and fuel composition
Thorium fuels		Well beyond FIT 1.0
“Both” means both metal/fast reactor/echem and oxide/fast reactor/UREX+1. Melt refining and AIROX are considered potential “minimum fuel treatment” examples.		

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## ACRONYMS

AIROX	Atomics International Reduction Oxidation
at%	atomic percent
Bk	Berkelium
BSG	Borosilicate glass
C	carbon
Cd	cadmium
Cf	californium
CFR	Code of Federal Regulations
Ci	curie
COEX	Co-extraction (of uranium and plutonium)
CR	transuranic conversion ratio
DOE	Department of Energy
DOT	Department of Transportation
DPL	Decision Programming Language
DSARR	Dynamic Systems Analysis Report for Nuclear Fuel Recycle
DU	depleted uranium
Echem	electro-chemical
EU	enriched uranium
FCF	Fuel Conditioning Facility
FCR&D	Fuel Cycle R&D, component of FCT program
FCT	Fuel Cycle Technology program
FFP	fraction of fission product
FIT	Fuel-cycle Integration and Tradeoffs
FP	fission product
FPEX	Fission Product Extraction
FR	fast reactor
FY	Fiscal Year
GDSE	Generic Disposal System Environment
GNEP	Global Nuclear Energy Partnership
Gr	group – one of 18 columns in the Periodic Table
GTCC	Greater-Than-Class C
HEU	highly enriched uranium



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HEPA	high efficiency particular air, a type of high-efficiency air filter
HLW	high-level waste
HM	heavy metal (thorium, protactinium, uranium, or transuranics)
HTGR	High Temperature Gas Reactor
HWR	Heavy Water Reactor
iHM	initial heavy metal, the heavy metal content prior to irradiation of fresh fuel
INL	Idaho National Laboratory
IWMS	Integrated Waste Management Strategy
LEU	lowly enriched uranium
LLW	low-level waste
Ln	Lanthanide
LWR	light-water reactor
MFT	Minimum Fuel Treatment
MLLW	mixed low-level waste
MOX	mixed oxide fuel
MW	megawatt
MWth	megawatt thermal
MWe	megawatt electric
NA	Not applicable
NE	nuclear energy
NUEX	Neptunium (and Plutonium) extraction
NU	natural uranium
ppm	parts per million
Pu	plutonium
PUREX	Plutonium Uranium Reduction Extraction
R&D	research and development
Rh	rhodium
Ru	ruthenium
RU	recovered uranium
SFR	Sweden Final Repository for radioactive operational waste, began operation in 1988
SNF	Spent Nuclear Fuel
SNM	special nuclear material
Si	silicon
SiC	silicon carbide

Sr	strontium
TALSPEAK	Trivalent Actinide Lanthanide Separation by Phosphoric Extractants and Aqueous Complexes
tbd, TBD	to be determined
T <sub>1/2</sub>	halflife
Tc	technetium
Th	thorium
TM	transition metal
TMFP	transition metal fission products
Tonne	metric ton, 1000 kg
TRISO	<u>Tr</u> istructural- <u>is</u> otropic, a type of micro fuel particle containing an oxide or oxycarbide kernel or fuel meat, surrounded by four layers of three isotropic materials - porous buffer layer of carbon, inner layer of dense pyrolytic carbon, ceramic layer of silicon carbide, and outer layer of dense pyrolytic carbon
TRU	transuranic element (neptunium, plutonium, americium, curium, berkelium, californium)
TRUEX	TransUranic Extraction
TRUMOX	transuranic-bearing MOX
U	uranium
UDS	undissolved solids
UOX	uranium oxide fuel
UOX-51	uranium oxide fuel taken to a burnup of 51 MWth-day/kg-iHM
UREX	Uranium Extraction
UREX+	Uranium Extraction-plus
U.S.	United States
U-TRU	uranium-transuranic
VB	Visual Basic
VISION	Verifiable Fuel Cycle Simulation mode
WA	Washington, site of a low-level waste near-surface burial waste disposal site
WAC	waste acceptance criteria
wt%	weight percent



# SYSTEM ANALYSIS CAMPAIGN SEPARATION CAMPAIGN FUELS CAMPAIGN THE FIT MODEL

## 1. OVERVIEW

The system losses study started in FY2009 [Shropshire2009] and continued through FY2010 [Piet2010a]. It became necessary to create a model for the team to use to (a) permit a systematic examination of the chemical behavior of a fuel cycle and (b) analyze cases. The FY2009 exploratory analysis was limited to equilibrium analysis of the fast reactor recycling loop at transuranic conversion ratio of 0.5, assuming incoming uranium and used LWR UOX-51 transuranic (TRU) streams were pure. In essence, the only specific impurity in fuel that received much attention was the set of lanthanides. In FY2010, it became clear that an analytical tool was required to consider a wider range of types of impurities and a wider range of technology options because the program was no longer focused on fast reactors fueled by used TRU from uranium oxide fuels. That model is called FIT, Fuel-cycle Integration and Tradeoffs. This report describes that model and how to use it.

This report documents the model. The FY2010 system losses report [Piet2010a] provides results and more of the basic observations gained from creating and using the model. The six topics in the system losses study report are as follows:

- Topic 1. The R&D program must improve chemical completeness and consistency
- Topic 2. Don't forget the uranium
- Topic 3. The full recycle strategy requires ...
- Topic 4. The modified open cycle strategy requires ...
- Topic 5. More complete dis-assembly of used fuel would have advantages, and costs.
- Topic 6. Broad R&D Questions

### 1.1 Purpose

FIT is a method to analyze different fuel cycles using common bases; in particular, to determine how changes in one part of a fuel cycle (say, fuel burnup, cooling, or reprocessing separation efficiencies) affect other parts of the fuel cycle. FIT provides the following:

- Rough estimate of physics and mass balance feasibility of combinations of technologies. If feasibility is an issue, it provides an estimate of how performance would have to change to achieve feasibility.
- Estimate of impurities in fuel and impurities in waste as function of separation performance, fuel fabrication, reactor, uranium source, etc.

A different way to describe the purpose of FIT is as a management, qualitative, and quantitative tool to integrate technical information in the FCR&D program.

## 1.2 Structure

Figure 1-1 illustrates the basic mass flows. It is the simplest framework on which we could base our analysis. Several user-defined inputs were fixed for the initial analysis – technologies and parameter ranges for which we had the most knowledge and for which individual parts of the calculation could best be validated. The incoming used fuel is always LWR UOX-51 in this report; users can input a different fuel. Separation of used UOX-51 provides the feed to start a recycle loop with a fast reactor, which is always a fast reactor with a transuranic conversion ratio of 0.50 in this report. Users can change the reactor in the recycle loop with some limitations described below.

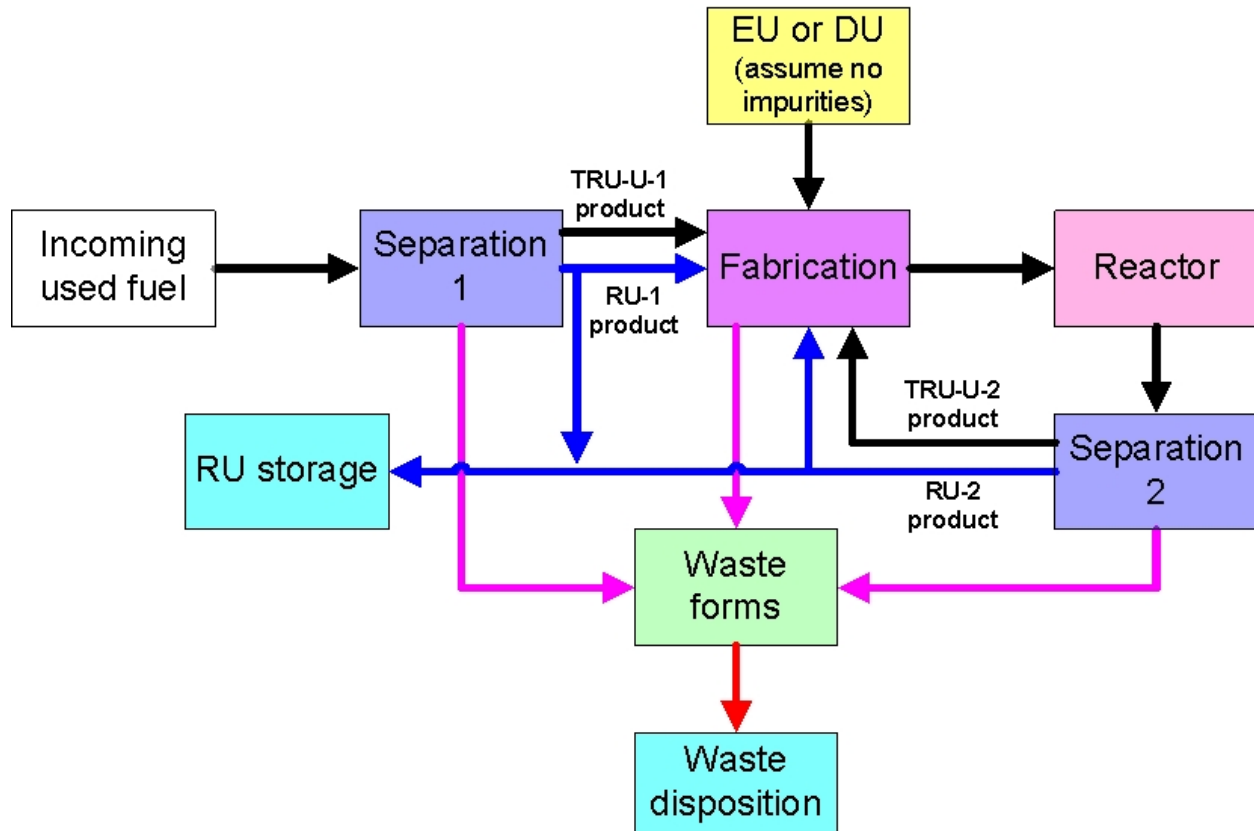


Figure 1-1. Basic mass flows; the quantitative tool does not yet address EU feed as an option.

For the first recycle iteration (recycle-1), there are only the streams from incoming used fuel via separation-1. There is no mass flow yet from separation-2. For subsequent recycle streams, the TRU-U-1 product mass flow from separation-1 remains as before and the TRU-U-2 product mass from separation-2 from the previous iteration is added to create a combined TRU-U product stream. The user selects whether to use RU-1, RU-2, or DU to blend with this combined TRU-U product stream. (The current model assumes an adequate supply of whichever source of uranium is used.). The model estimates the required ratio of TRU-U product to U feed for that recycle's iteration. Since the TRU-U product can contain uranium, and the RU streams will typically contain some TRU impurity, the ratio of TRU-U product to U product is not the same as the chemical TRU:U ratio in the final blended product.

Figure 1-2 shows a preliminary assessment of choices (green) and information flows (red) on top of the mass flows (black). Team discussion made it obvious that no two people viewed the information steps the same (i.e., what decisions lead to what outcomes). That realization generated the need for a “solver” or “optimizer” that will be able to use the mass flow engine from different perspectives. That solver does not yet exist.

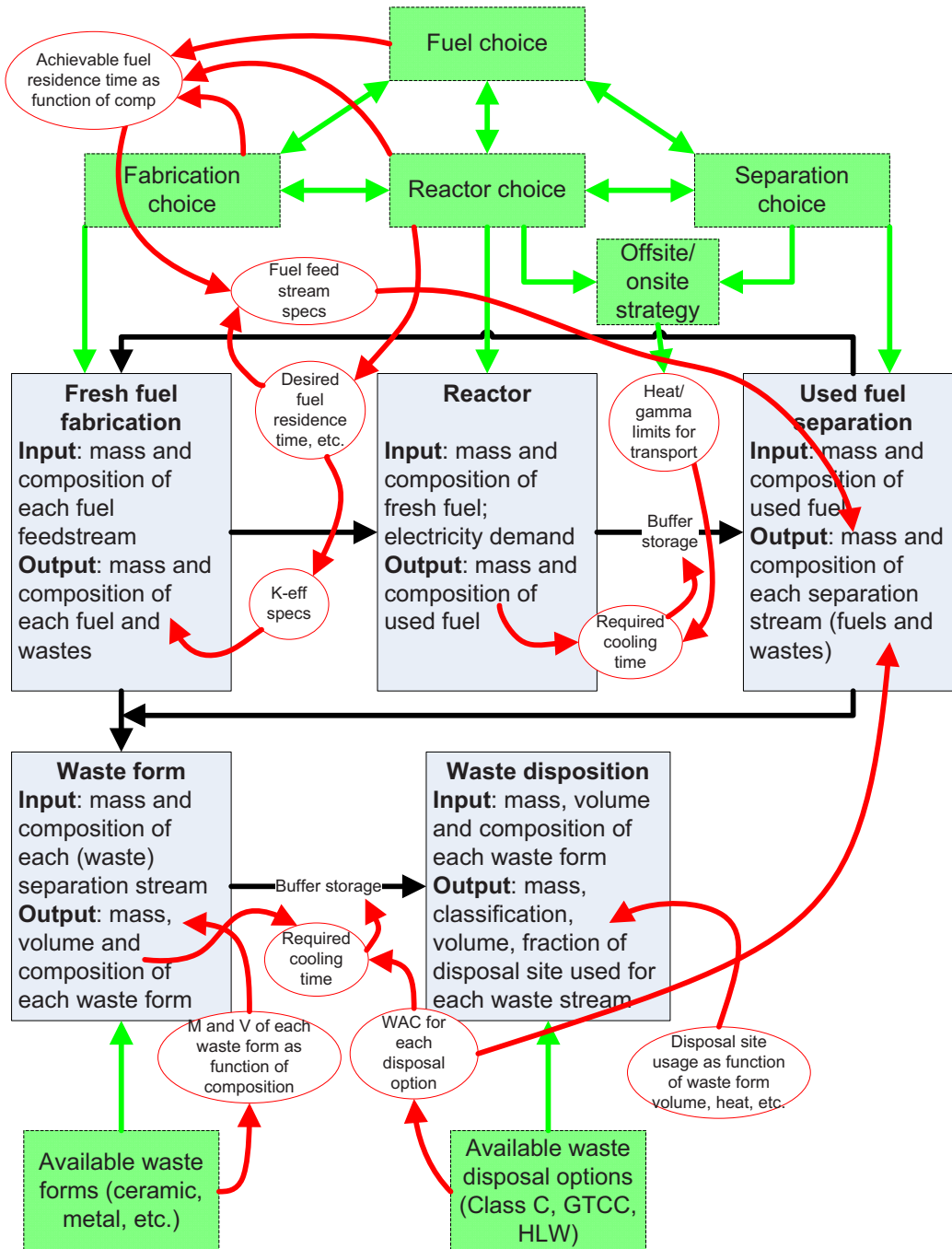


Figure 1-2. Technological choices (green) and information flows (red) overlaying mass flows (black).

FIT requires a PC with Excel2007. Installation (Chapter 2) results in three key files on your PC, together with various auxiliary files that the typical user will not need to consider:

1. FIT Excel2007 file
  - o Current version is FIT 1.0.xlsm
2. Mrtrauwinery Excel2007 file

- Current version is mrtauWinery\_v-05.xlsm
3. MRTAU.exe FORTRAN executable file (this does not require a FORTRAN compiler)
    - Current version is MRTAUvs1a.exe

The FIT file controls everything. It performs all calculations (and associated data) other than the physics and blending calculations, i.e., the fraction of TRU-U feed versus uranium feed. FIT calls the MrTauWinery Excel2007 file for blending before fuel fabrication. After fuel fabrication, it again calls the MrTauWinery Excel2007 file, which this time uses the MrTau FORTRAN file for a depletion calculation to get the actinide part of the output composition.

It calls and links to the MrTauWinery Excel2007 file, which itself calls the FORTRAN executable. MrTau is a standalone physics tool described elsewhere.[Bays2010a, Bays2010b] Users only need to open the MrTauWinery Excel2007 file if they wish to add or change physics data or change the method of 1-group cross sections that control the blending ratios between separation-1, separation-2, and DU.

If a new version of MrTauWinery Excel2007 or FORTRAN is created, it can be placed in the MRTAU directory (created during installation). When FIT is run, the user simply gives it the new name of the Excel2007 file.

## 1.3 Limitations and Assumptions

Users should understand the following limitations and assumptions.

### 1.3.1 Physics

FIT uses “reference” fuel compositions that must be calculated in some other fashion, such as those in the Transmutation Library [Piet2010a]. The model needs two fuel compositions – that of the incoming stream and that for the reactor in the recycle loop. The composition of the incoming stream is used, as is. FIT adjusts the composition of the reference fuel in the recycle loop according to what happens in the simulation.

The blending calculation in MrTauWinery to make the fuel in the recycle loop requires that the “k” of the fuel composition to be made must equal to the “k” of the original “reference” fuel, with the implication that the resulting fuel could have the same fuel residence time – from the physics perspective.

1-group cross sections are used to make the input fuel composition adjustment noted above. This occurs in MrTauWinery, combining methods described elsewhere.[Yee2008, Bays2009, Bays2010a, Bays2010b] As impurities appear or fuel isotope compositions change criticality from the feedstock assumed in the “reference” fuel calculations, the model adjusts the TRU:U ratio accordingly.

- FIT 1.0 does not have the option of using enriched uranium as one of the feeds to the recycle loop.

MrTauWinery is also used to calculate the recycle loop’s reactor discharge composition according to the adjusted input composition.

- Adjustment by adding impurities in one or more feeds.
- Adjustment of the TRU:U ratio as noted above.
- Adjustment by impurities that may occur during fuel fabrication.

The depletion part of MrTau does not yet account for fission products, i.e., does not calculate fission products in the depletion model. Until it does, FIT approximates fission products in the recycle loop fuel discharge as follows:

- Fission products in the input stream are carried into the output stream with no impact from fuel irradiation. In FY2011, we will estimate the importance of this by using FY2010 independent results from E. Hoffman [Hoffman2010] but preliminary analysis indicates it has little impact.
- Fission products created during the fuel irradiation are (well) approximated by the fission products in the original reference fuel output composition.

This depletion calculation is essentially a simplified version of ORIGEN equations and is done by the FORTRAN executable invoked by the MrTauWinery Excel2007 file.

Radionuclide decay is accounted for in various storage steps in the FIT model. FIT uses a simplified decay calculation. Most of the tracked radionuclides that have a half-life of greater than 4000 years are considered stable for the purposes of this model. In FIT, the user can specify a decay time for each of the storage steps. Entering a number storage time of greater than 400 years will result in some significant error in the decay calculation. Therefore, FIT is limited to calculating storage steps of less than 400 years.

### 1.3.2 Feed stocks

The default incoming used fuel composition is LWR UOX at 51 MWth-day/kg-iHM burnup, aged 15 years. The user can change the aging time from 0 to 30 on the worksheet Input\_Sep1. The user can change the fuel composition by substituting new data on the worksheet UOX-51 raw data, but in the exact same format and without changing the worksheet name.

There are four data columns in the MrTauWinery Excel2007 file allowing compositions for the recycle loop's reactor. These are currently as follows:

- Fast reactor, metal fuel, CR=0.5, startup composition (case 14)
- Fast reactor, oxide fuel, CR=0.5, startup composition (case 15)
- Fast reactor, metal fuel, CR=0.5, equilibrium composition (case 16)
- Fast reactor, oxide fuel, CR=0.5, equilibrium composition (case 17)

These can be changed, but the model assumes that cases 14 and 16 are metal fuel and 15 and 17 are oxide fuel. That assumption determines which fuel fabrication models (metal or oxide) are used.

RU-1 comes from separation-1; RU-2 comes from separation-2. The compositions are calculated in the model.

The composition of DU is set in MrTauWinery Excel2007 file. The values there correspond to 0.2% tails<sup>b</sup> and no impurities. Users can change the values to match other assumptions.

The user selects on the Control worksheet whether to use RU-1, RU-2, or DU. We recommend RU-1 for the first recycle iteration (there is no RU-2 for recycle-1) and RU-2 for subsequent recycles, corresponding to keeping all the U with TRU in fast reactor recycling. The supply of the selected source

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<sup>b</sup> To calculate mass balanced and composition when uranium is enriched, one has to specify the U-235 content in both in the enriched product and in the residual depleted uranium. The former is determined by reactor physics. The latter is called "tails" and is based on economics. Common practice is in the range 0.2% to 0.3%. We have been using 0.2%; the user can input whatever they wish.



of uranium is unlimited in FIT 1.0. This is a fine assumption for non-breeder reactor cases as there is always excess uranium in the system.

### 1.3.3 Separations

The separation efficiencies are assumed static as the composition changes, e.g., as impurities accumulate. So, if 0.5% of the lanthanides are indicated as going into fuel, that percentage is constant regardless of how high the lanthanide impurity in the fuel may grow.

The model has four separation data sets corresponding to UREX+1a, electrochemical, AIROX, and melt refining.[Piet2010b] These can be changed. These are matrices. The rows are the isotopes, elements, and groups of elements tracked in FIT. The columns are the output products, both fuels and wastes. Each value tells the spreadsheet what fraction or percent of that isotope/element/group goes into that column's product.

### 1.3.4 Fuel fabrication

There are no models for recycle of materials for non-fuel use, e.g., lanthanides for use in solar or wind (nuclear-assisted solar or wind energy), zirconium for new cladding, or graphite blocks.

The composition of fuel is not constrained by impurity limits. The model uses various inputs to calculate the level of impurities in fuel and in waste; the user has to determine if the levels of impurities are acceptable and, if not, what inputs must be changed to search for an acceptable combination of parameters.

Fuel impurity limits can be expressed as the limit of an impurity in finished fuel product, in the blended composition going into fuel fabrication, or in one or more of the feeds to be blended during fuel fabrication. Any of these are typically parts per million (ppm), but the (unstated) denominator basis varies (fuel, fuel feed, or a particular fuel feed). Note that the working Fuels Campaign limits are specified in terms of the TRU feedstock with four key assumptions.

1. The TRU feed stream was only TRU.
2. The uranium blended to make fuel is assumed chemically pure. Thus, the "DU feed" calculations best match the underlying Fuels Campaign assumptions.
3. The fast reactor has a TRU conversion ratio near 0.5. The conversion ratio determines the ratio of TRU:U.
4. No significant impurities enter during fuel fabrication itself.

Thus, for system losses study purposes, these had to be back-calculated to determine impurity limits on the final fuel product.

Fuel impurity limits for a given element or set of elements can arise from one or more of the following:

- Impact on fuel matrix performance during irradiation
- Impact on fuel – cladding (or coating) interaction during irradiation
- Impact on fuel fabrication
- Increase in neutron absorption (this is approximated in FIT)

- Displacement of fuel (this is not addressed in FIT because the team felt it would be easily adjusted for).

Many current Fuels impurity limits are groups of elements, some of which are fission products and some are not. Our available data on fuel composition only includes fission products. FIT is set up to address non-fission products.

The working Fuels impurity limits stem from consideration of what impurities might be present from mining, milling, etc. - but not fission products that would be formed while in the reactor.

### 1.3.5 Waste management

Waste management is addressed in the model by tracking the masses of all materials separated from used fuel that are not recycled into new fuel. Waste streams generated during fuel fabrication are also tracked. Users can also track operations and maintenance wastes generated during separations, although operations and maintenance wastes created in other parts of the fuel cycle (the front end, initial fuel fabrication, the reactors) are not yet included in this model.

The waste streams are treated in the model so as to convert the waste stream into a waste form suitable for disposal. The waste forms used in the model are generally consistent with the recent studies of the Integrated Waste Management Strategy (IWMS, Gombert 2008), the Advanced Fuel Cycle Facility (AFCF) design (DOE 2007), and the Waste Form Campaign (Vienna 2010). This results in waste classification (or at least ultimate waste disposition) presumptions regarding what waste form is required or desired for which waste disposition.

The user may rely on the waste classification interpretations used in the referenced IWMS, AFCF design, and Waste Form Campaign studies that are based on minimal variation from how current waste policies and regulations are interpreted. Or, the user may use the characteristics of the waste streams to make assessments about how some waste streams could be managed. In some cases, assumptions used in the model may not be consistent with some interpretations of current, source-based waste management policy and regulations. In some cases, the waste form may be more robust than required if that waste stream is managed according to its hazard characteristics. Most important, we track and report the waste characteristics and the presumed waste forms, so the user can, if he desires, assess how the waste forms can be appropriately managed. The model includes various options for placing different waste streams into different optional waste forms.

We also presume in the model that waste mass and volume reduction will be important. So, especially for the high-volume and high-mass wastes from separations process operations and maintenance, we presume the use of thermal treatment to not only convert the waste stream to a robust waste form that should meet storage, transportation, and disposal requirements, but also to significantly reduce the waste form volume and mass compared to other options, such as grouting. This approach is based on the presumption that more rigorous waste treatment may be desired to reduce waste volume and mass. Reducing the volume and mass of the large amounts of operating and maintenance wastes can show stakeholders how closed fuel cycle options not only recover and recycle valuable fissile and fertile material from used fuel, but also how these options use state of the art technologies to minimize radioactive wastes generated during fuel recycling.

FIT 1.0 does not yet include up-to-date assumptions about waste packaging and void space, although the framework in the model allows those updates in the future and allows the user to modify current placeholders.

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## 2. INSTALLATION

Installing FIT 1.0 requires a PC running Microsoft Excel2007. Perform the following steps to install FIT 1.0:

- Copy the FIT 1.0.xlsm file to your local hard drive from the CD-ROM or flash drive. The location is not important.
- Copy the “MRTAU” folder with its contents to the C drive on your PC at the root level (i.e. C:\). The location of the “MRTAU” folder is important.

The main file in the “MRTAU” folder is “mrtauWinery\_v0-5.xlsm”. This is the file that FIT interacts with when performing a simulation. Open the FIT 1.0.xlsm file and go to the first worksheet “Control”. If prompted, allow Excel2007 to execute macros. Verify that the filename in cell “C2” matches the MRTAU filename “mrtauWinery\_v0-5.xlsm”. These need to match or FIT will not be able to interact with MRTAU to perform depletion calculations.

Simulations are executed from the **Control** worksheet. Select parameters in blue and radio buttons to set up simulation. Run the first iteration by pressing the Run first iteration button. Change any necessary parameters, and enter the number of subsequent iterations desired (n). Then press Run iteration loop to execute the iterations 2 through n.

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### 3. INPUTS AND DESCRIPTION OF EACH WORKSHEET

Start by opening the FIT file and going to the left-most worksheet, called **Control**. With the exception of physics data and reference input/output composition data, all data and settings are in the FIT Excel2007 file, which is described next. The physics data and input/output composition options are in the MrTauWinery Excel2007 file, which is described after FIT.

#### 3.1 In the FIT Excel2007 File

The top part of the **Control** worksheet is the main control panel, where the basic settings are selected and the user runs either recycle-1 (the first iteration) or a designated number of iterations after recycle 1.

The bottom part of the **Control** worksheet is a set of navigation buttons (Table 3-1) that takes the user to the indicated worksheets. One can of course also go to those worksheets by selecting the worksheet at the bottom of the Excel2007 file.

Table 3-1. Navigation choices on **Control** Worksheet (color coded in the FIT Excel2007 file).

General	Separation1 related calculations	Fuel Recipe adjustment calculations	Oxide fuel fabrication	Metal fuel fabrication	Reactor/input-output	Separation2 related calculations	Waste processing calculation	Waste disposal calculations
Control	UOX-51 raw data	Fuel Input Adjustment	Inputs	Inputs	Reactor output	Separation2 calculation	Inputs	Heat and dose data
Output	Input for Separations 1		Isotopic blending	Feed preparation	Reactor storage	Separation2 storage	Recovered uranium	Waste disposition selection
Model Flow	UREX+1a calculations		Manufacturing process	Manufacturing process			Zeolite	Waste storage
	Separation matrices		Scrap recovery process	Scrap recovery process			Glass bonded zeolite	Waste final disposal output
	Separation1		QC testing	QC testing			Lanthanide glass	
	Separation1 storage		Summary output	Summary output			Kr/Xe	
			Fuel fabrication storage				Cs/Sr	
							Metal alloy ingot	
							Remainder metal	
							Grout	
							Solvents-Liquids	
							Fuel fabrication wastes	
							Operational wastes	
							HLW glass output	
							HLW glass input	
							HLW glass calculations	

### 3.1.1 Control

First, make any data changes to this file and/or MrTauWinery Excel2007 file.

Second, make any changes to the settings on the **Control** worksheet.

- **MRTAU filename:** user types in the name of the MrTauWinery Excel2007 file you wish to use.
  - Default = mrtauWinery\_v0-5.xlsm
  - If you want to change the composition of incoming fuel, go to worksheet **UOX-51 raw data**. If you want to change the aging of the incoming fuel, go to worksheet **Input\_Sep1**.
- **Separations 1:** drop down list, options are UREX+1a, ECHEM, AIROX, melt refine
- **Separations:** Material from Separations 1 or Material from both separations
  - **Sep1 storage:** the number of years between separations 1 and when fuel is blended and inserted into the reactor
- **Reactor:** drop down list, options are
  - Fast reactor, metal fuel, CR=0.5, startup composition
  - Fast reactor, oxide fuel, CR=0.5, startup composition
  - Fast reactor, metal fuel, CR=0.5, equilibrium composition
  - Fast reactor, oxide fuel, CR=0.5, equilibrium composition
- **Rx storage:** the number of years between reactor discharge and when fuel is enters separation 2.
- **Separations 2:** drop down list, options are UREX+1a, ECHEM, AIROX, melt refine
  - **Sep2 storage:** the number of years between separations 2 and when fuel is blended and inserted into the reactor
- **Number of iterations:** input the integer number of iterations you wish FIT to calculate. It will not take many to cause the system's chemistry to stabilize. To date, we have used 9 or 19 to be conservative. For example, 19 iterations plus the first iteration gives a total of 20.

Third, run the calculation.

- For recycle 1, select Material from Separations 1 and click on Run first iteration.
- For recycle > 1, select Material from both separations and click on Run iteration loop.

### 3.1.2 Separation 1

These worksheets provide the incoming material for the recycle loop and have several inputs the user may wish to review or change.

- To change the type of incoming fuel, the composition on the **UOX-51 raw data** worksheet must be changed.

- To change the aging of the incoming fuel (time from reactor discharge to input to separations1), use the worksheet **Input\_Sep1**.
- To change the separation efficiencies for electrochemical, AIROX, or melt refining, go to the worksheet **Sep\_Matrices**.
- To change the separation efficiencies for UREX+1a, go to the **UREX+1a** worksheet.

**UOX-51 raw data** contains the detailed isotopic data for LWR UOX-51. In FIT 1.0, if the user wants to change the incoming fuel type, these data must be replaced with the new fuel type. However, the name of the worksheet must not change and the exact format on this page must be maintained. In particular, a defined range “UOX\_Table” must be unchanged.

**Input\_Sep1** prepares the feed stream into separation1. Of particular note is cell T2, which controls the length of time that the incoming feed material is aged. This is a pull down menu, not a number input field. The user must select one of the possible aging periods corresponding to a column on the **UOX-51 raw data** worksheet as the spreadsheet uses a “lookup” function to pull the appropriate data from that worksheet.

The worksheet **UREX+1a** calculates the separation factors for UREX+1a based on the split fractions from Candido Periera, Continuous Lab-Scale Separations Factors from 2009 Research, personal communication to Layne Pincock, 27 May, 2010. Where separation factors are missing or 100%, default values of 99.9% to desired product and 0.1% to waste are used.

The worksheet **Sep\_Matrices** contains the matrices that take each tracked isotope or chemical element or group of chemical elements and provides the percentage that goes to each product or waste stream. The totals for each row must equal to 100% or mass is lost.

- UREX+1 data are pulled from the worksheet **UREX+1a**.
- Electrochemical (echem) data are input here. Data in the file now come from G. Teske.
- AIROX data are input here. Data in the file now come from Christianson1999.
- Melt refine data are input here. Data in the file now come from G. Teske.

**Calc\_Sep1** calculates the inventory going to each of the output separation streams based on the split factors in the worksheet **Sep\_Matrices** and based on the user input of the selected separation process. The columns on the left bring in the reactor output stream. The user-selected options on the **Control** worksheet and the values on worksheets **UREX\_1a calculations** and **separation matrices** are copied to the block on this page called “separation 1”. The separation matrix then produces the separations output mass streams further to the right. Cell J34 should read “Mass is balanced”. If not, there is an error with the separation matrix.

For the separations calculation, there is a check box entitled “UDS goes to Glass (UREX+1a)”. The default is to have this unchecked. If it is selected, the undissolved solids (UDS) would be combined with the raffinate/residual in the HLW glass waste form. If it is unchecked, the UDS would then go into the metal alloy ingot waste form.

Cell H21 allows the user to select what percent of the fuel meat (except for volatile fission products, noble gases, halogens, C<sup>14</sup> and H<sup>3</sup>) becomes UDS for UREX+1a only.

There is also another check box entitled “Lanthanides combine with HLW glass”. The default is to have this unchecked. If it is checked the lanthanides would then be combined with the raffinate/residual in the



HLW glass waste form. If it is unchecked the lanthanides would then go into a lanthanide glass waste form.

These check boxes also show up on worksheet **Calc\_Sep2**, and they are linked together. If the user checks them, then it checks them in both places and affects separations1 and separations2.

**Sep1\_Storage** calculates the input spent fuel inventory change (due to decay and in-growth) for the specified number of years of storage between separations and fuel fabrication. There are three blocks of data, but “U-TRU product 2” is not currently being used. “From Sep 1” brings into the page the output from separation-2. Cell M2 displays the numbers of years of storage between separation2 and fuel blend/reactor input, this value is input on the **Control** worksheet, not here! The length of storage is used to calculate the aged composition, which is then used in the blending and fuel fabrication calculations.

### 3.1.3 Fuel input adjustment

There no user inputs on this worksheets.

This worksheet calculates what goes to the fuel input adjustment calculation in the MrTauWinery Excel2007 file. If the user has selected Material from Separations 1 on the **Control** worksheet, it simply uses the mass flow from separations1. If the user has selected Material from both separations, it adds the mass flows from separations1 and separations2. The input composition adjustment in MrTauWinery requires mass fractions, so mass fractions are calculated from the total mass flow. The mass fractions returning from MrTauWinery are then converted into moles as input to fuel fabrication.

### 3.1.4 Oxide fuel fabrication

Reject rate projections are input on the **Inputs\_O** worksheet, i.e., the percent of input mass flow that leads to reject product at each step in fuel fabrication. In the other worksheets the fraction of the reject rate going into various waste streams (recycle, container waste, HEPA waste, etc) is a user input.

More information on the various steps in fuel fabrication can be found in the system losses study report.

The **Inputs\_O** worksheet is the start of the oxide fuel submodel within FIT, provided by Eric Shaber and Melissa Teague. However, the original submodel’s calculation of the TRU:U ratio is over-ridden because that is calculated in FIT on the **Fuel Input Adj** worksheet. Column V has the total reject rate for the various steps in the fuel fabrication process, which can be changed by a knowledgeable user.

**Feed Prep** calculates the preparation stream.

**Iso Blend\_O** calculates stoichiometric adjustment from making metal nitrate and later denitration.

**Process\_O** has the details of fuel fabrication.

**QC Test\_O** details quality control testing of fuel.

**Recovery\_O** describes what in-processes wastes are recovered and sent back to feed preparation.

**Summary\_O** provides summary information for metal fuel fabrication. Information and masses proceed to worksheet **Fuel Fab\_Storage**.

### 3.1.5 Metal fuel fabrication

Reject rate projections are input on the **Inputs** worksheet, i.e., the percent of input mass flow that leads to reject product at each step in fuel fabrication. In the other worksheets the fraction of the reject rate going into various waste streams (recycle, container waste, HEPA waste, etc) is a user input.

More information on the various steps in fuel fabrication can be found in the system losses study report.

The **Inputs** worksheet is the start of the metal fuel submodel within FIT, provided by Eric Shaber and Melissa Teague. However, the original submodel's calculation of the TRU:U ratio is over-ridden because that is calculated in FIT on the **Fuel Input Adj** worksheet. Column AA has the total reject rate for the various steps in the fuel fabrication process, which can be changed by a knowledgeable user.

**Feed Prep** calculates the preparation stream.

**Process** has the details of fuel fabrication.

**QC Test** details quality control testing of fuel.

**Recovery** describes what in-processes wastes are recovered and sent back to feed preparation.

**Summary** provides summary information for metal fuel fabrication. Information and masses proceed to worksheet **Fuel Fab\_Storage**.

### 3.1.6 Fuel fab storage (the last step before reactor input)

There no user inputs on this worksheets.

For metal fuels (cases 14 or 16 in MrTauWinery), this worksheet draws from metal fuel fabrication. For oxide fuels (cases 15 or 17 in MrTauWinery), this worksheet draws from oxide fuel fabrication.

**Fuel Fab\_Storage** calculates the reactor input fuel composition for the specified number of years of storage after fuel fabrication. Cell K2 has the number of years of storage between fuel fabrication and insertion into the reactor. The years of decay is set to a default of zero years in this version of FIT so that the model does not have to perform another fuel input adjustment (as discussed in 3.1.3). This is assuming that the fuel is fabricated just in time to be inserted into the reactor. (A delay of a month or so would make no significant difference. A delay of a year would be significant, in which case in the current model a year would have to be added to the time lag between separation and fuel fabrication.) The length of storage is used to calculate the composition that goes into the reactor, which is then used in **Reactor\_Output**.

This worksheet will be simpler once MrTauWinery calculates both actinides and fission products. Currently, the input in kg/year is partitioned into the actinides that are sent to the MrTau depletion calculation and the fission products or other impurities that pass directly into the output fuel composition. So, this worksheet calculates the total mass of actinides and fission products respectively.

### 3.1.7 Reactor

There no user inputs on these worksheets.

**Reactor\_Output** brings the output composition as calculated by MrTauWinery Excel2007 file back into the FIT spreadsheet and reassembles the total mass reactor output mass flow. This worksheet will be simpler once MrTauWinery calculates both actinides and fission products. Currently, the output composition is assembled as follows.

- The actinides (kg/yr) are calculated by the output mass fractions from MrTauWinery times the total mass of actinides from worksheet **Fuel Fab\_Storage**. Note that the mass fraction sent to MrTauWinery is 1.00. MrTauWinery then returns a total mass fraction less than 1.00, the difference is the mass of the actinides fissioned into fission products.

- The fission products are assembled from two sources. One source is the fission products in the input fuel. The total mass of those fission products was calculated on worksheet **Fuel Fab Storage** and is shown here in cell D11. Those fission products are brought into column H without change, i.e., neutron irradiation changes to existing fission products are ignored because they are generally small, especially from the chemical standpoint. We will re-examine their importance in creating or transmuting each long-lived isotope. The second source is the fission products created from fission of the fuel during this pass in the reactor.
  - The total mass of actinides going into the reactor is given by 'Fuel Fab\_Storage'!AB33 and shown on this worksheet in cell D7.
  - The total mass of actinides returning from the reactor as calculated by MrTauWinery is the sum of the output vector in row2, shown here in cell D8.
  - The inferred mass of fission products stemming from actinide fission is the difference, shown here in cell D9. That mass is multiplied by the fission product composition in the original/reference fuel output composition, which has been copied by a macro from MrTauWinery Excel2007 file into column L. Those values have to be renormalized in column M because the original mass fractions are fractions of 1 unit of input fuel, i.e., there are both actinides and fission products summing to 1.00. These mass fractions will be multiplied by the mass of new fission products and so the sum of mass fractions of the fission products alone must sum to 1.00.
- The support ratio from the incoming fuel and the reactor in the recycling loop is calculated in cell K10. This is not currently output each recycle iteration.

**Reactor\_Storage** calculates the input spent fuel inventory change (due to decay and in-growth) for the specified number of years of storage after irradiation in the reactor. Cell K2 has the numbers of years of storage between reactor output and input to separation2, this value is input on the **Control** worksheet, not here! The length of storage is used to calculate the aged composition, which is then used in separation2.

### 3.1.8 Separation 2

There no user inputs on these worksheets.

Separation information should be input on worksheets **UREX\_1a calculations** and **separation matrices**.

**Calc\_Sep2** calculates the inventory going to each of the output separation streams based on the split factors in the worksheet **Sep\_Matrices** and based on the user input of the selected separation process. The columns on the left bring in the reactor output stream. The user-selected options on the Control worksheet and the values on worksheets **UREX\_1a calculations** and **separation matrices** are copied to the block on this page called “separation 2”. The separation matrix then produces the mass streams further to the right. Cell J34 should read “Mass is balanced”. If not, there is an error with the separation matrix.

**Sep2\_Storage** calculates the input spent fuel inventory change (due to decay and in-growth) for the specified number of years of storage between separations and fuel fabrication. There are three blocks of data, but “U-TRU product 2” is not currently being used. “From Sep 2” brings into the page the output from separation2. Cell M2 has the numbers of years of storage between separation2 and fuel blend/reactor input, this value is input on the **Control** worksheet, not here! The length of storage is used to calculate the aged composition, which is then used in the blending and fuel fabrication calculations.

### 3.1.9 Waste Streams

The FIT model includes the necessary blocks for tracking waste streams separated from used fuel during recycling and produced during recycle fuel fabrication. Operating and maintenance wastes for separations and fuel fabrication are also included; but operating and maintenance wastes from front-end processes, the first (LWR) reactor, and the recycle reactor are not included in the model at this time. If these presently-excluded waste streams are determined through future analyses to be potentially significant in analyzing different fuel cycle options, then they may be included in future versions of FIT.

The model is designed to enable user-selected waste treatment options that are defined to meet user-intended waste dispositions that could dictate what treatments, waste forms, and waste loadings are needed. The model adopts waste forms that are generally consistent with recent studies of the Integrated Waste Management Strategy (Gombert 2008), the Advanced Fuel Cycle Facility (AFCF) design (DOE 2007), and the Waste Form Campaign (Vienna 2010).

Potential waste streams and waste forms in this version of the model are summarized in Table 3-2. The different separations processes do not produce all of these waste streams; zero values are present in the model structure for waste streams that are not produced in that specific separations process. Masses and volumes of the waste forms are calculated based on waste loadings of the waste forms, consistent with models developed by the Waste Form Campaign for glass (Ryan 2009) estimations made by the Integrated Waste Management Strategy, the AFCF, and the Waste Form Campaign. Waste packaging, and the impacts on waste volumes and masses introduced by waste packaging, are not yet included in the model structure.

#### 3.1.9.1 Carbon-14

The model includes the following assumptions and estimates as input or bounding conditions.

- Carbon, in fuel meat of either oxide or metal fuels, present as either an impurity or fission product, will partition differently for some different separations processes. (FIT is set up to track both C-14 and C-other. There is nil C-other as a fission product, so data are needed regarding the amount of other carbon from processing fluids.) Any amount of carbon that evolves to process gas streams, regardless of the separations process, is presumed to eventually oxidize to gaseous CO<sub>2</sub> that requires capture and retention in a solid waste form for disposal. In reality, regulatory emission regulations for C-14 may enable regulatory-compliant atmospheric discharge of any gasified C-14 (Soelberg 2009, Vienna 2010). The model accounts for the more conservative possibility that 90% of the gasified carbon is quantitatively captured (after oxidation to CO<sub>2</sub>) using a caustic scrubber, and stabilized in a solid calcium carbonate grout. (Carbonates of magnesium and sodium are also possibilities that are not included in this model.) The value of capture efficiency can be varied by the user.
- High levels of contamination by stable carbon in CO<sub>2</sub> contributed from air or by other process materials could dilute the amount of radioactive CO<sub>2</sub> from the used fuel, and proportionately increase the amount of the CaCO<sub>3</sub> waste form. The AFCF study assumed a 100x dilution factor (and corresponding 100x increase in the CaCO<sub>3</sub> waste form) from CO<sub>2</sub> in process air (DOE 2007).
- C14 is assumed to partition quantitatively to the recovered U stream and the undissolved cladding and metal stream in electrochemical separations. In this case, no separate grouted C14 waste stream is assumed; no dilution from tramp CO<sub>2</sub> from air is assumed, since the electrochemical separations process is performed in an inert Ar atmosphere; and the C14 is just one of many isotopes that are impurities in the recovered U and fission products in the electrochemical metal

waste form. The electrochemical metal waste form contains most of the Tc and lesser amounts of other fission products that do not dissolve in the electro refiner molten salt bath.

- Carbon, as a trace constituent in metal cladding and structural materials, remains with those metals if those metals are not dissolved during a separations process. Carbon in metals that are dissolved would partition to the process stream that contains those metals.
- Carbon in carbon-based or SiC-based cladding, fuel element, and core structure, is either oxidized to gaseous CO<sub>2</sub> if those materials are oxidized; or if those materials are not combusted, then the carbon partitions to the process stream that contains those carbon-based materials. These materials are not present in the current version of the model because it is not yet tailored for use cases that include graphite or SiC-based cladding, fuel elements, or core structures that would exist in HTGR or MSR reactors.

Table 3-2. Waste streams and waste forms in the FIT model.

Separated waste isotope(s)	From these separations processes	Waste form	Comments
C14	All except electrochemical	Grouted carbonate	Based on longevity and potential mobility; free release may be allowed (Waste Form Campaign current reference case)
I129 (and co-collected halogens)	All	zeolite	Based on longevity and potential mobility
Tc99, UDS	UREX+1	Metal ingot	Based on longevity and potential mobility. Could be combined with HLW glass.
Tritium	All	Grouted Tritiated water	Generally accepted disposition, although disposition as HLW may still be required; or free release may be allowed after sufficient decay prior to separations
Kr85 (and other Kr and Xe isotopes)	All	Compressed gas	Free release after sufficient decay time
Cladding, UDS, baskets	Electrochemical	Metal ingot	Combined with Tc99 metal
Raffinate/residual	All but electrochemical	Glass	Could include Tc, UDS, Cs/Sr, and lanthanides in aqueous separations
Raffinate/residual (salt waste)	Electrochemical	Glass-bonded zeolite	
Cs/Sr	UREX+1	Mineralized monolith	Could (or may be required to) be combined with HLW glass, depending on waste policy interpretation or economics
Lanthanides	UREX+1	Glass	Could be combined with HLW glass
Cladding/coatings	Aqueous	Compacted	Presumes residual TRU contamination >10 nCi/g
Structure/hardware	All	Compacted	Presumes combined with Cladding/coatings
Spent solvents-liquids	UREX+1	Mineralized monolith	Presumes TRU can be reduced to <10 nCi/g
Fuel fabrication wastes	---	Compact	
Operations and maintenance wastes	All	Mineralized monolith	Presumes some wastes contaminated with TRU >10 nCi/g
Operations and maintenance wastes	All	Mineralized monolith	Presumes some wastes with TRU <10 nCi/g

### 3.1.9.2 I129 and other halogens

The model includes the following assumptions and estimates as input or bounding conditions.

- I129 and other halogens are assumed to partition almost quantitatively to process gas streams in all but electrochemical separations, during which it partitions almost quantitatively to the glass-bonded ceramic fission product waste stream.
- Nearly quantitative capture of I129 is assumed to be necessary to meet air emission limits. Even the trace amount of I129 (0.1 wt% of the total I129) that is assumed to partition to process gas

streams during electrochemical separations is assumed to be captured to meet air emission limits. The I129 and other halogens are quantitatively captured in the model using silver-impregnated zeolite sorbent, which is the final waste form (the Separations and Waste Form Campaigns are also studying alternative sorbents and waste forms). The Ag-zeolite waste form is assumed to have a waste loading of 2.53 wt% for total halogens.

### **3.1.9.3 Tc99**

Technetium behaves differently in the different separations processes in this model. The model includes the following assumptions and estimates as input or bounding conditions.

- UREX+1 separates most of the Tc into a separate waste stream that is combined with Zircalloy (from cladding) and stainless steel (from fuel assembly structural steel) into a melted metal waste form that contains not more than 5 wt% Tc.
- The Tc is assumed to not dissolve in electrochemical separations and so remains with cladding, other metals, and other fission products, inert materials, or contaminants that do not dissolve into the molten salt bath of the electro refiner.
- These electro refiner UDS are purified a separate melter that removes and recycles remaining fission product salts, and melts the UDS into a metal ingot. This mass is combined with the mass of the Tc metal waste form from UREX+1 separation for storage and disposal.
- Tc is assumed to nearly quantitatively partition to the fission product waste stream in AIROX separations.
- Tc is assumed to mainly remain with the U-TRU product during melt refining, although 8% of the total Tc is assumed to partition to the fission product waste stream.

### **3.1.9.4 UDS from UREX+1 separations**

Fuel meat materials that do not dissolve in the dissolver are may be either combined with the Tc into a metal waste form or combined with other FPs in a glass waste form. The user can determine this. Both the metal and glass waste forms have loading limits for the amount of this UDS, so this UDS can affect the final mass of those waste forms.

### **3.1.9.5 Tritium**

Tritium is assumed to evolve quantitatively to process gas streams in all separations processes. The amount that can be discharged to the atmosphere, within regulatory limits, varies depending on air dispersion and process facility size. The model assumes that 99% of the tritium requires capture, and 1% can be released. In all separations cases, the tritium is assumed to be converted to tritiated water, which is captured using standard industrial molecular sieve technology. The molecular sieve is thermally regenerated, and the captured tritiated water removed from the mole sieve is condensed and grouted into a solid waste form. The waste loading of tritium is 0.106 wt%, because of dilution of the tritiated water with tramp water in the different processes or with water added to raise the moisture content of the process gas to a level at which 99% of the total water can be captured in the mole sieve.

### **3.1.9.6 Noble gases**

Noble gases including Kr85, the only significant radioactive noble gas fission product (at waste management time scales), will almost quantitatively evolve to the process gas streams in all separations

processes. These gases are captured onto a zeolite sorbent, and desorbed and compressed into gas cylinders for storage and disposal.

### **3.1.9.7 Cladding and baskets from electrochemical separations**

The cladding and baskets that are used to hold the fuel in the electro refiner do not dissolve. The electro refiner UDS are purified a separate melter that removes and recycles remaining fission product salts, and melts the UDS into a metal ingot. This mass is combined with the mass of the Tc metal waste form from UREX+1 separation for storage and disposal.

### **3.1.9.8 “Raffinate/residual” fission product wastes**

For simplicity, the waste stream from any of the separations processes that contains the majority of the fission products is called, after the UREX+1 nomenclature, as “raffinate/residual” wastes. These waste streams from all but electrochemical separations are vitrified into a glass waste form based on the glass waste form model used in FIT.

The fission product-bearing electro refiner salt from electrochemical separations is stabilized in a glass-bonded zeolite waste form. The maximum assumed FP waste loading is assumed to be 5 wt%.

### **3.1.9.9 Lanthanides from UREX+1 separations**

UREX+1 can separate the lanthanides from other product and waste streams. These lanthanides can be converted in the model into either a lanthanide glass or total combined fission product glass waste form, with or without UDS that did not dissolve in the dissolver, using the glass model in FIT.

### **3.1.9.10 Cladding and coatings from all but electrochemical separations**

The cladding, and coating for fuel are assumed to be separated from the used fuel in all separations processes. In all but electrochemical separations, metal cladding can be combined with Tc and other metal and converted to a metal Tc waste form. Cladding metal and any non-metallic cladding/coatings that are not otherwise used or oxidized to process gases are decontaminated (to a limited degree) and compacted into a final waste form.

### **3.1.9.11 Fuel assembly structure and hardware**

Fuel assembly structure and hardware is expected to have activation products and possibly have some contamination of fission products, and will require handling as radioactive waste or products. This metal is cut away from fuel assemblies before the fuel rods are chopped, to minimize contamination. The metal can be added to cladding and Tc to make a Tc metal waste form. Any metal left over can be compacted and discarded as radioactive waste.

### **3.1.9.12 Cs/Sr from UREX+1 separations**

UREX+1 can separate the Cs/Sr (and other Group 1A/2A isotopes) from the other waste and product streams. While the Cs/Sr waste stream can be combined with fission products and converted to a glass waste form (as is done in the other separations processes) this waste stream can also be converted to an aluminosilicate waste form for separate handling, storage, and disposal. The maximum expected waste loading is about 31 wt%, but this value does not consider limitations due to decay heat generation.



### 3.1.9.13 Spent solvents and liquids from UREX+1 separations

The complex UREX+1 separations process includes multiple steps and multiple solvents and extractions. The organic solvents degrade over time due to radiation damage to the organic molecules. Fresh solvents are added to enable spent solvents to be discharged. These liquid streams are thermally treated in the model to reduce both the mass and volume of the final waste form, and to convert the waste into an aluminosilicate waste form suitable for disposal. Through thermal treatment, the waste mass is reduced by about 100x.

### 3.1.9.14 Fuel fabrication waste streams

Several waste streams are created from fuel fabrication. The streams included in this model for mixed oxide fuel fabrication are shown in Table 3-3. The solid waste streams (Iso Blend waste, container wastes, HEPA wastes, scrap, other solids) are presumed to contain the same isotopic proportions as are in the final fuel, for simplicity. These waste streams are compacted and packaged for final disposition.

Table 3-3. Mixed oxide fuel fabrication waste streams from worksheet "Summary\_O".

<b>FUEL WASTES</b>	
Fuel From Iso Blend (g)	<b>926</b>
<b>Fuel From Process</b>	
Container Waste (g)	<b>9,075</b>
HEPA Filter Waste (g)	<b>8,445</b>
<b>Fuel From Recovery</b>	
Container Waste (g)	<b>1,139</b>
HEPA Filter Waste (g)	<b>83</b>
Fuel From QC Testing (g)	<b>1,042</b>
<b>PROCESS BY-PRODUCTS</b>	
<b>Fuel Iso Blend HEPA Exhaust</b>	
Hydrogen	<b>20,374</b>
NO3	<b>1,253,366</b>
Water	<b>1,274,538</b>
<b>Fuel Process Wastes</b>	
HEPA Filter Solids (g)	<b>0</b>
Gaseous Discharge (g)	<b>1</b>
<b>Recovery Process Wastes</b>	
Scrap Fuel Cladding and Fines (g)	<b>319</b>
Chemical Solids (SIC, Tramp Matl.) (g)	<b>5,270</b>
Waste Water (g)	<b>46,592</b>
<b>QC Testing Wastes (g)</b>	
Gaseous Discharge through HEPA's	<b>10,502</b>
Process Water & Acids	<b>0</b>
Mercury	<b>54</b>
Metallograpy Compounds	<b>967</b>

<b>FUEL WASTES</b>	
Fuel From Iso Blend (g)	<b>926</b>
<b>Fuel From Process</b>	
Container Waste (g)	<b>9,075</b>
HEPA Filter Waste (g)	<b>8445</b>
<b>Fuel From Recovery</b>	
Container Waste (g)	<b>1,139</b>
HEPA Filter Waste (g)	<b>83</b>
Fuel From QC Testing (g)	<b>1,042</b>
<b>PROCESS BY-PRODUCTS</b>	
<b>Fuel Iso Blend HEPA Exhaust</b>	
Hydrogen	<b>20,374</b>
NO3	<b>1,253,366</b>
Water	<b>1,274,538</b>
<b>Fuel Process Wastes</b>	
HEPA Filter Solids (g)	<b>0</b>
Gaseous Discharge (g)	<b>1</b>
<b>Recovery Process Wastes</b>	
Scrap Fuel Cladding and Fines (g)	<b>319</b>
Chemical Solids (SiC, Tramp Matl.) (g)	<b>5,270</b>
Waste Water (g)	<b>46,592</b>
<b>QC Testing Wastes (g)</b>	
Gaseous Discharge through HEPA's	<b>10,502</b>
Process Water & Acids	<b>0</b>
Mercury	<b>54</b>
Metallograpy Compounds	<b>967</b>

### 3.1.9.15 Separations process operations and maintenance wastes

Separations process operations and maintenance wastes will include contaminated personal protective equipment (PPE) for radiation workers, decontamination solutions, filters, and spent and discarded tools and equipment, including process equipment and hot cell maintenance wastes. Metallic wastes are decontaminated to the extent practical, compacted, and packaged for disposal. Inorganic filters and frames are leached to decontaminate and recover TRU and fission products, and compacted.

Liquid and organic wastes can be significantly volume-reduced by thermal treatment, incineration, evaporation, etc. These are volume-reduced by about a factor of 100x, and mass-reduced by a factor of 10x, and stabilized in an aluminosilicate waste form.

Considering the volume and mass reduction of the organic and liquid wastes, the potential contamination on spent/discarded tools and equipment suggests that a portion of these wastes may be contaminated with TRU elements at levels that make them candidates for subsurface geologic disposal.

## 3.2 In MrTauWinery Excel2007 File

MrTauWinery is a standalone physics tool. Therefore, most of the spreadsheet should not be changed by a FIT user. Indeed, many parts of the tool are not used by FIT. The parts of the MrTauWinery Excel2007 file of interest to the FIT user are described in the following sections.

Indeed, the input adjustment parts of MrTauWinery Excel2007 file have 20 cases, primarily intended for stand-alone use of this file. Four of the cases have been utilized for FIT purposes. None of the formats can be changed. But, the data in these cases can be changed for FIT purposes. These cases and their current contents are as follows:

- 14 = Fast reactor, metal fuel, CR=0.5, startup composition
- 15 = Fast reactor, oxide fuel, CR=0.5, startup composition
- 16 = Fast reactor, metal fuel, CR=0.5, equilibrium composition

17 = Fast reactor, oxide fuel, CR=0.5, equilibrium composition

### 3.2.1 Calc input adjust (FP)

The user should not change anything on this worksheet.

When this file is used as a standalone tool, the parallel worksheet, **Calc input adj**, is used. For FIT purposes, this worksheet, **Calc input adjust (FP)**, is used. Unlike the former, it allows for composition adjustment of impurities and isotopes, as well as three types of uranium, RU-1, RU-2, or DU.

Cell Q1 is provided by FIT; it selects among the three uranium cases.

Cells L86, M86, and N86 are the percentages of RU-1, RU-2, and DU used to make the uranium composition used in making the final TRU-U blend. At present, the only values that will appear in these cells are 0% and 100%, with 100% being which type of uranium the user selected in FIT. That is, the model does not allow for the possibility that the supply of RU-1 or RU-2 would be insufficient or for a deliberate blending of RU-1 and RU-2. The user can replace the values in these cells and break the link to the cell Q1, however, they must still total to 100%.

Cells Q89 and S89 are the calculated required blending of the TRU-U and U products respectively. Since both products can have uranium, TRU, and impurities, these blending percentages are not the same as the TRU:U in the finished product. Those numbers are in column V. Cell V10 is the fraction of uranium, cell V34 is the fraction of TRU, and cell V84 is the fraction of impurities.

### 3.2.2 Initial recipes

The user can change cases 14 through 17 to run FIT with different compositions corresponding to other than CR=0.5 fast reactors. However, the formats must not change.

Note that there are three blocks of rows. The user must have self-consistent data in all three blocks.

- The block of rows called Input mass fractions has the fractions of input fuel composition (must total to 1.0 or mass is lost or created)
- The block of rows for Output mass fractions has the fractions of output fuel composition (must total to 1.0) with a set of 81 isotopes, elements, and groups of elements.
- The block of rows called Output mass fractions (set of 92) is the same as the block of rows called output mass fractions, except that there is a slightly different grouping of elements. We inadvertently have both sets of groupings used in FIT. The FIT Excel2007 file uses the set of 81 and the worksheet **calc input adj (FP)** uses the set of 92.

### 3.2.3 Available material

The user should not change anything on this worksheet.

FIT places the available TRU-U product isotopic data into column B.

### 3.2.4 Available uranium

There are three columns for RU-1, RU-2, and DU. These are used by “calc input adjust (FP)”. When MrTauWinery is used as a standalone tool, the user may change any of these columns of data. However, when MrTauWinery is used with FIT, the user can only change the DU column. If the user changes RU-1

or RU-2, they will be written over by copy and paste operations by FIT, in which the appropriate RU-1 and RU-2 compositions calculated by FIT are inserted here.

### **3.2.5 Cross sections**

In the stand-alone tool, the user would select the data she wanted to have in column B. With FIT, the user selects among cases 14-15-16-17 and FIT copies that column's data into column B.

Column B is used by **worksheet calc input adj(FP)** and is copied by FIT into the **budep.inp** worksheet for use by the FORTRAN executable.

Therefore, if cases 14-15-16-17 are altered by the user, the appropriate cross sections must be entered into those columns.

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## 4. OUTPUTS

Most of the output data a user would want is found on the **output** worksheet in FIT. Few of the worksheets have output information that the user would tend to want. A few possible exceptions are noted below.

The output data are simply numbers; the user must graph or compare them to impurity limits as he or she sees fit. For example, there is a Excel2007 file that compares the cases run in September 2010 to the current Fuels Campaign working limits and graphs them, see section 4.2.

### 4.1 Output Worksheet

Table 4-1 lists the information provided in the output worksheet. For example, if one wants to consider the composition of fresh fuel in the recycling reactor, use mass flows, to recycling reactor, columns LI to OL.

Table 4-1. Information available on the **Output** Worksheet.

Category	What parameters	Which Columns
Reactor burnup	Percent of HM input to the recycling reactor that is fissioned	IB
Reactor power	The power of the recycling reactor supported each iteration (The incoming fuel via separation1 is normalized to 1 GWe)	ON
Blending fractions	% TRU % U <i>Caution: these are the blending fractions of TRU-U product (combined from TRU-U-1 and TRU-U-2) and uranium product (from RU-1, RU-2, or DU). These are not the TRU:U compositions in the fuel, which must instead be obtained by mass fractions or mass flows, see below.</i>	BE BF
Mass fractions (by isotope or element)	Available TRU-U material (before blending with U) Adjusted composition (after blending with U)	BH to EU EW to HZ
Mass flows (by isotope or element)	To recycling reactor (after fuel fabrication) Out of recycling reactor (to separations2)	LI to OL ID to LG

Table 4-1. Information Available on the **Output** Worksheet (continued).

Category	What parameters	Which Columns
Waste management (totals for each parameter for each tracked isotope, element, and group of chemical elements.)	Heat (W/yr), Gamma (W/yr), neutron (W/yr), neutron number (#/s per year), radiotoxicity (Sv/yr) at t=0, radiotoxicity (Sv/yr) at t=10,000 years after reactor discharge, Mass (kg/yr), Volume (m <sup>3</sup> /yr)	HLW – C to J LLW class A/B/C – L to S Mixed LLW – U to AB LLW from decayed storage – AD to AK Mixed LLW from decayed storage – AM to AT LLW-GTCC – AV to BC
Waste management (kg/yr, m <sup>3</sup> /yr)	Zeolite Glass bonded zeolite Kr Xe Cs-Sr Metal alloy ingot Remainder metal HTO grout C14 grout Spent LLW organic solvents Other organic LLW Spent decon solution Waste water and acetic acid TRU-contaminated LLW Fuel fabrication wastes Operational wastes Operational wastes (TRU) HLW glass	OP-OQ OS-OT OV-OW OY-OZ PB-PC PE-PF PH-PI PK-PL PN-PO PP-PQ PR-PS PT-PU PV-PW PY-PZ QB-QC QE-QF QH-QI

## 4.2 Comparison with Impurity Limits

There are three steps required to compare FIT 1.0 outputs with Fuels Campaign Limits.

1. Fuels limits on TRU feedstock must be translated into limits on the final fuel product. This was done in FY2009 for metal and oxide fast reactor fuels.[Shropshire2009]
2. Split or allocate the grouped elements (e.g. Mo-Ru-Rh-Pd) in the FIT output to individual elements.
3. Re-group individual elements according to how elements are grouped in whichever fuel impurity limits you are considering.

The file “FIT Graphs 201-09-10.xlsx” does the second and third steps for the cases in the system losses report.

- Raw data from the FIT **output** worksheet are pasted into columns through DZ. Note that there are several hidden columns at present.
- Cells EH 1 to FD 2 allocate TM-other and Mo-Ru-Rh-Pd to individual elements. These fractions come from analysis of the fission product splits in fast reactor output compositions in the Transmutation Library.
- The columns EJ to FD then re-group elements to match the grouping in the oxide and metal fuel limits.

### 4.3 Other Information in FIT

Of course, all data at every step of the calculation in FIT can be found within the FIT or MrTauWinery Excel2007 files. However, except for the data copied and pasted into the **Output** worksheet, only the data for the most recent recycle iteration will be elsewhere in the FIT or MrTauWinery Excel2007 files. If these data are useful for a user, we can add them to the macro that copies and pastes data into the **Output** worksheet.

#### 4.3.1 Input data

Column A of the **Output** worksheet displays the settings that were selected on the **Control** Worksheet.

#### 4.3.2 Fuel fabrication

For oxide fuel, worksheet **Summary\_O** provides for oxide fuel fabrication such as scrap streams, fuel recovery, overall process efficiency.

For metal fuel, worksheet **Summary** provides summary information for metal fuel fabrication such as scrap stream masses, fuel alloy returned to melter, etc.

#### 4.3.3 Waste management

This model separately tracks the mass, volume, and isotopic content of each waste stream. This version of the model also presumes classification of waste streams into Class A/B/C, GTCC, mixed low-level, and HLW streams, based on current regulations and policies (NRC 2001, NRC 2009, NWSA 1982) and is generally consistent with the primary waste management reference sources [the Integrated Waste Management Strategy (IWMS, Gombert 2008), the Advanced Fuel Cycle Facility (AFCF) design (DOE 2007), and the Waste Form Campaign (Vienna 2010)].

Future versions of the model can include calculations of decay heat, radiotoxicity, and gamma and neutron emissions. Future versions can also track partitioning of TRU and FPs to spent solvent and operations/maintenance waste streams, to compare these parameters to Class A, B, and C LLW limits, and to estimate how much of the TRU and FPs will be lost in all of the different waste streams. This will be important in enabling assessment of how to disposition waste streams based on their risk rather than based on their source.



### 4.3.3.1 Waste Stream Outputs in FIT

Each of the waste streams whose inputs are listed in Section 3 of this report are tracked on worksheets in the Excel file. Figure 4-1 shows the tables for the grouted tritium and C14 waste forms. In these cases, no other isotopes are presumed to contaminate these waste forms.

Captured Gases		
44	H3	0.002490088 kg/yr
45	C14	7.12999E-07 kg/yr
46	C-other	0 kg/yr

HTO Grout	
Hydrogen	
Mass	2.49E-03 kg/yr
Waste Loading	0.106% mass waste per mass total
Waste Form Mass	2.35 kg/yr
Bulk Density	2.3 g/cm <sup>3</sup>
Volume	0.00102 m <sup>3</sup> /yr

C14 Grout	
Carbon	
Mass	7.13E-07 kg/yr
Waste Loading	12.00% kg/yr
Waste Form Mass	0.00001 kg/yr
Bulk Density	2 g/cm <sup>3</sup>
Volume	2.971E-09 m <sup>3</sup> /yr

Figure 4-1. Illustration of the tritium and C14 waste form output page on worksheet **Grout** in the model.

In other cases, the isotopic content is tracked from the separations processes based on the separation factors for the different isotopes, as shown in Figures 4-2 and 4-3 for the glass waste form. These figures show that the glass model from the Waste Form Campaign (Ryan 2009) is executed in FIT.

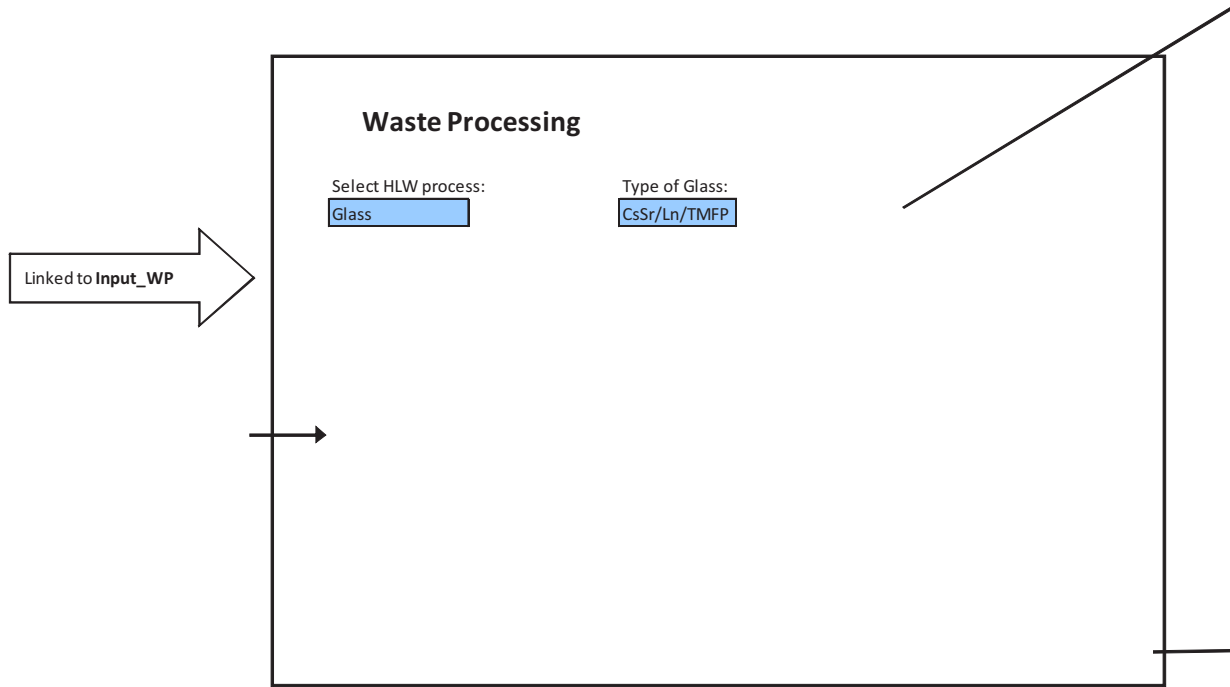


Figure 4-2. Glass waste form model execution calculation worksheet **Calc WP** in the Excel2007 file.

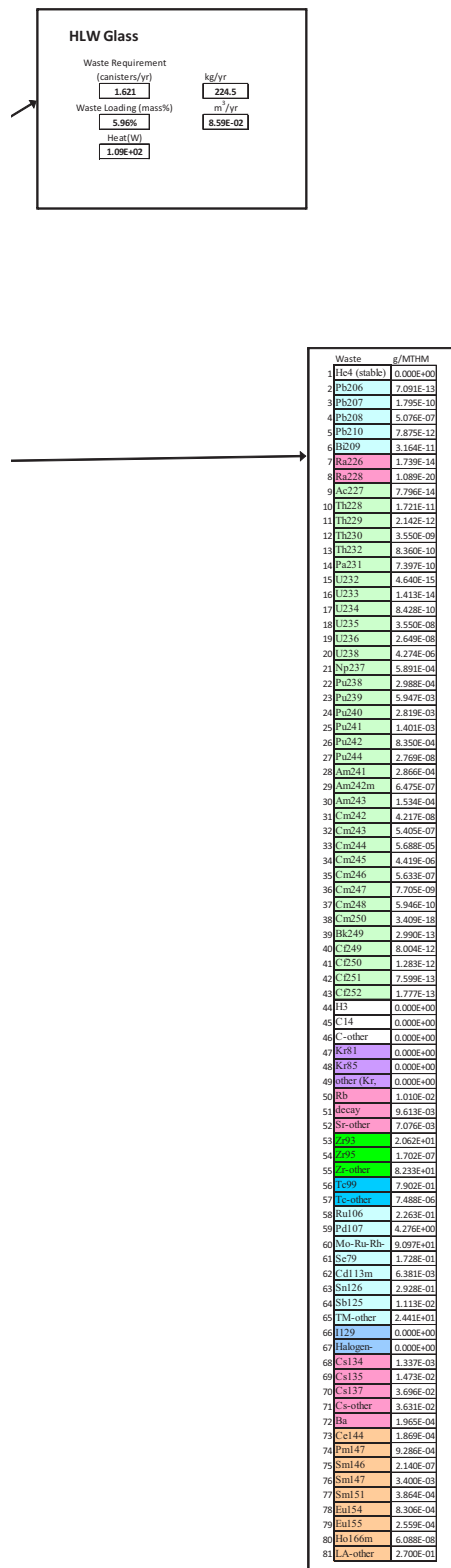


Figure 4-3. Calculation of glass waste form parameters and isotopic content in the worksheet **Calc WP** in the Excel2007 file.

#### 4.4 Other Information in MrTauWinery Excel2007 File

Worksheet **Calc input adj (FP)** has the calculated “k” value for the targeted or reference composition of the reactor and fuel in the recycle loop. This worksheet can also be consulted to determine how much of the neutron absorption or fissions come from which element.

Worksheet **available uranium** has the RU-1 and RU-2 compositions in the last iteration of FIT.

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## 5. FUTURE WORK

We invite feedback and suggestions for future work. Of course, plans must evolve as program priorities and budgets change.

### 5.1 Current Plans for FY2011

FIT in the current FY2011 budget. The workscope is to make it a more user-friendly version. Some of the items intended for FY2011 subject to priorities and budgets are as follows:

In the system analysis tools budget, we plan to create a version of MrTauWinery that incorporates fission products. That should eliminate the fission product approximations used in FIT/MrTauWinery at present.

We must harmonize the inadvertent selection of different sets (81 versus 92) sets of isotopes, elements, and groups of chemical elements in different parts of FIT and MrTauWinery. This is probably the time to track each second row transition metal. Mo-Ru-Rh-Pd would be tracked individually. TM-other would be split into Nb, In, Sb, Te, Se and a remainder. This would make comparison with Fuels limits more straightforward and more accurate. Both “splits” are more complicated than they may seem because isotopes of each element decay into other elements. So, the set of tracked isotopes will have to be re-examined to determine if more isotopes must be included.

FIT should calculate the supply of RU-1 and RU-2 and FIT should not use more than in supply.

The waste processing module needs further refinement and review. There are missing pieces of data that need a referenceable source.

We should add data quality indicators to the data we have and any new data, likely on a 1-5 scale:

1. Source of data is industrial-scale testing or operation
2. Source of data is pilot-scale testing or operation
3. Source of data is continuous lab-scale testing or operation
4. Source of data is batch lab-scale testing or operation
5. Source of data is estimates from subject matter experts, averages from other elements, or default values).

We should make it easier to add more reactor/fuel composition cases.

The input and data matrices should be adjusted so that as data on impurities from processing are available, they can be added.

### 5.2 Next tier of needs for FY2011 if resources permit

Economic calculations could be added to FIT under the economic analysis work packages.

After gathering more data, we could add a calculation of the number of containers to waste output.

Various additives for each separation process still need to be gathered and entered into the model (solvents, salts, etc, especially for electrochemical).

We could add a suite of standard analysis graphs as an automatic output from FIT so that the users do not have to generate their own output graphs manually.

### 5.2.1.1 Waste Characterization

At present, the user must select a waste classification for each waste stream. This has two problems. First, the model uses current waste classification names, which may or may not exist in the decades to come.

Second, it does not allow for different classification for waste streams on the basis of changing criteria or changing waste stream composition. We should replace the manual waste classification with one that asks users for the criteria to judge waste classification and then have FIT automatically assign each waste stream on the basis of its composition. Possibilities include the following:

- < 100 nCi of alpha-emitting TRU (half-life greater than 20 years) per gram of waste – per 40CFR191
- < 100 nCi of alpha-emitting TRU (half-life greater than 5 years) per gram of waste – per 10CFR61
- Specific isotope concentration limits (Ci/g or Ci/m<sup>3</sup>) in 10CFR61, defining low-level waste class C suitable for near-surface burial in 10CFR61.
- Specific isotope concentration limits (Ci/g) extended to other isotopes not in 10CFR61 by S. A. Fetter [Fetter1988, Fetter1990]
- Heat limitation (W/kg of waste form, W/m<sup>3</sup> of waste form, or W/m<sup>3</sup> of packaged waste) as suggested by Kocher and Croff [Kocher1987] and the Nuclear Energy Agency [NEAR2006] as a possible characteristic-based dividing line between waste classes.
  - 2000 W/m<sup>3</sup> - apparently based on long-term geologic disposal complications [NEA2006]
  - 50 W/m<sup>3</sup> - based on heat complications in near-surface burial situations [Kocher1987]
  - 700 Ci/m<sup>3</sup> for all isotopes with half-life less than 5 years [10CFR61]. This is intended to guard against excessive difficulties from contact dose or heat during handling and emplacement of the waste.
- IAEA waste classification schemes.

The above examples illustrate the complexity of this task because there are different possible criteria, expressed in different units. But, it also shows the potential value for automating the task. In theory, as the losses of TRU into waste are small, there may be no waste that is simultaneously high-heat and high longevity for radiotoxicity.

Table 5-1 shows how radioactive wastes might be considered based on their levels of decay heat (which challenges the durability and performance of the waste form, waste packaging, storage sites, and long-term disposal systems) and long-term radiotoxicity (which indicates the hazard that needs to be isolated by the waste form, waste packaging, storage sites, and disposal sites).

Table 5-1. Radioactive waste characterization based on decay heat and long-term radiotoxicity (Bays 2010c).

	High Long-Term Radiotoxicity	Low Long-Term Radiotoxicity
High Heat	<p>Example isotopes: Transuranics (and Trans-thorium).</p> <p>Expected disposition: Deep geological disposal, none of which presently exist.</p>	<p>Example isotopes: <math>^3\text{H}</math>, <math>^{85}\text{Kr}</math>, <math>^{137}\text{Cs}</math>, <math>^{90}\text{Sr}</math>.</p> <p>Example disposition: de facto decay during storage of used fuel in the U.S. while the fuel awaits either final disposal.</p>
Low Heat	<p>Example isotopes: <math>^{14}\text{C}</math>, <math>^{99}\text{Tc}</math>, <math>^{129}\text{I}</math>.</p> <p>Example disposition: Waste entombed in decommissioned U.S. nuclear facilities, German Konrad Mine.</p>	<p>Example isotopes: Shorter lived fission products in low concentrations.</p> <p>Example disposition: Shallow land burial in the U.S. of waste that meets current Class A, B, or C LLW limits.</p>

High decay heat, high long-term radiotoxicity wastes (such as spent nuclear fuel, and waste streams from separating used fuels that contain the majority of fission products and TRU isotopes that are not recycled) are those wastes that would require disposal in geologic repository systems that will isolate these wastes from the environment for geological timeframes. Such repositories do not yet exist in the U.S. so there is presently considerable uncertainty in how we will isolate these waste streams, which is an issue for the public acceptance of the nuclear fuel cycle.

High decay heat, but low long-term radiotoxicity wastes could include some waste streams that contain relatively short-lived fission products such as  $^3\text{H}$ ,  $^{85}\text{Kr}$ ,  $^{139}\text{Cs}$ , and  $^{90}\text{Sr}$ , separated from used fuel (and other, long-lived isotopes) in some potential separations processes. These waste streams might be best disposed through a combination of a decay storage for time duration long enough so that levels of residual radionuclides meet Class A, B, or C LLW or mixed LLW concentration limits, after which they can be disposed at relatively low cost as low-heat, low radiotoxicity, *low-risk* wastes. Uncertainty, cost, and risk in how these wastes can be disposed are lower than for high heat, high radiotoxicity wastes. The current de facto decay during storage of used fuel in the U.S. for up to 50 years (and more every year that storage continues), while the fuel awaits either final disposal or closure of the nuclear fuel cycle, provides a precedent for this approach, which has gained public and regulatory acceptance. MIT 2010 recommends storage of used fuel for about 100 years to allow decay of short-lived isotopes.

Low decay heat, but high long-term radiotoxicity wastes could include some wastes presently classified as GTCC, and waste streams that contain minor actinides that are separated from used fuel but not recycled for some fuel cycle options. These kinds of waste streams, (following decay storage of short-lived isotopes, if needed) may still require isolation for geological timeframes, but not necessarily in waste forms, packages, and disposal sites that are designed to tolerate high decay heat. Uncertainty, cost, and risk in how these wastes can be disposed *are lower* than for high heat, high radiotoxicity wastes. Precedents of how these types of wastes are disposed exist in the U.S. and other countries (such as entombment of radioactive materials in decommissioned and buried DOE facilities, and the Waste Isolation Pilot Plant in the U.S., and the Konrad Mine in Germany [Bandt2003, Sailer2008]).



Low decay heat, low radiotoxicity wastes could include waste streams now classified under current regulations as Class A, B, or C LLW. Existing LLW disposal sites are precedents of safe and relatively low cost disposal of these kinds of wastes in the U.S. and other countries.

### 5.2.1.2 Fuel impurity limits

At present, the user must manually compare fuel composition with postulated Fuel impurity limits. One could automate this process by asking the user to supply Fuel impurity limits and then automatically comparing them. This has one major complication, which is that until and unless there are data for all elements in a limited chemical group, it could be seriously misleading. For example, consider a limit on all halogens. F and Cl are present only from processing impurities. Br and I will be present because they are fission products; they could also arise as processing impurities. If there are no data on process-source impurities, then comparing Br and I to the total halogen limit (and finding it acceptable) could give a false sense of security.

Another complication with fuel impurity limits is that the rationale for impurity limits varies. Furthermore, if a design fix were implemented to relax one of the limits, there could be another limit that would come into play, i.e., it would not be appropriate to assume the element would become unlimited. For example, consider a limit on lanthanides because of their impact on fuel-cladding interactions. This limit would be relaxed or eliminated if a new cladding or barrier between fuel and cladding were added (with attendant costs); but rather than become unlimited, the lanthanides might then become limited by some other consideration on the following list.

- Impact on fuel matrix performance during irradiation
- Impact on fuel – cladding (or coating) interaction during irradiation
- Impact on fuel fabrication
- Increase in neutron absorption (this is approximated in FIT)
- Displacement of fuel (this is not addressed in FIT because the team felt it would be easily adjusted for).

The relevance to FIT is that we may invite the user to separately input a limit based on one or more of the above categories of constraints. Then, allow the user to deactivate all the limits of a given category in which case the remaining limits would apply.

## 5.3 More Advanced Possibilities

Add an option for enriched uranium (EU).

Add an option for natural uranium (NU).

Add an option to turn off the separation-1 stream (as required for a breeder calculation).

Add thorium fuel cycles as an option, this would require an update to MrTau.

Develop and test an “optimizer” or “solver” that would iteratively and automatically run the mass flow engine to balance criteria or to meet a particular criterion.

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- 10 CFR 63 Nuclear Regulatory Commission, "Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada," Title 10, Part 63 of the Code of Federal Regulations, revised as of 2002.
- 40 CFR 191 Environmental Protection Agency, "Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes," Title 40, Part 191 of the Code of Federal Regulations, revised as of 2002.
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