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Best-Basis Inventory Maintenance Tool (BBIM): Database Description and User Guide

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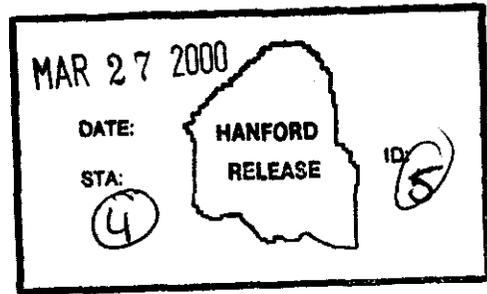
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**BEST-BASIS INVENTORY MAINTENANCE TOOL (BBIM):
DATABASE DESCRIPTION AND USER GUIDE**

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LIST OF TERMS

Auto TCR	Automated Tank Characterization Report
BBIM	Best Basis Inventory Maintenance Tool
BBIMCOMBO	a software program that connects users to the BBIM database application; the data entry process
Ci	Curies
Ci/L	Curies per liter
Ci/mL	Curies per milliliter
CONFIGMGNT	Configuration Management
g/mL	grams per milliliter
HDW	Hanford Defined Waste
IC	ion chromatography
ICP	inductively coupled plasma
ID	identification
Kgal	kilogallon
kL	kiloliter
M	molar
mCi/L	microcuries per liter
mg/L	micrograms per liter
RPD	relative percent difference
TWINS	Tank Waste Information Network System
uCi/g	microcuries per gram
uCi/mL	microcuries per milliliter
ug/g	micrograms per gram
ug/l	micrograms per liter
ug/mL	micrograms per milliliter
wt%	weight percent
wt% C	weight percent carbon

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1.0 INTRODUCTION

The **Best Basis Inventory Maintenance Tool (BBIM)** is a computer database application with built-in calculations that model the chemical composition of the Hanford tank wastes in terms of three fundamental parameters:

1. Analyte concentration
2. Waste density
3. Waste volume

Using these parameters, the BBIM is able to calculate for all of the Best-Basis constituents in each of the 177 tanks:

1. Total tank waste inventories
2. Phase-based inventories
3. Phase-based concentrations

Calculations are handled differently depending upon the pedigree or type of the underlying data; for example, the input concentration could be in solid units, such as "ug/g" or in liquid units, such as "ug/mL". In each of these cases, there would be slight variations to the basic inventory calculation formula (Concentration * Density * Volume).

In addition to calculating inventories, the BBIM also documents the source of the underlying data and how the calculations were performed.

An enhancement is planned for 1Q00 to account for wastes transferred between tanks. When this is in place, the BBIM will be able to reflect ongoing Tank Farm operations, and will continuously (with a slight lag behind operational activities) maintain the documented best-basis inventory.

1.1 DOCUMENT ORGANIZATION

Chapters	Name	Description
2-3	Introduction to the BBIM Calculations	<ul style="list-style-type: none"> • For the user who wants to know how the BBIM models the waste. • How the calculations are done.
4-5	BBIMCOMBO	<ul style="list-style-type: none"> • Entering, reviewing, approving the data
6	CONFIGMGNT	<ul style="list-style-type: none"> • Publishing to TWINS
7	Technical Description	<ul style="list-style-type: none"> • Database tables, data models, algorithms, etc.
App. A	Definition of Terms	<ul style="list-style-type: none"> • Glossary of terms used in the document
App. B	Computation Rules and Formulae	<ul style="list-style-type: none"> • More detail on how the calculations are performed
App. C	Entity-Relationship Diagram	<ul style="list-style-type: none"> • Most important tables and relationships in the BBIM

1.2 BBIM SYSTEM COMPONENTS

The BBIM System consists of several major components as described in Table 1-1. These components work together to provide the ability to enter data, review the calculated results, publish data into the public view via TWINS and via the Auto TCR, run several predefined queries and reports, and create many ad-hoc queries in support of ongoing site operations such as Waste Retrieval and Privatization.

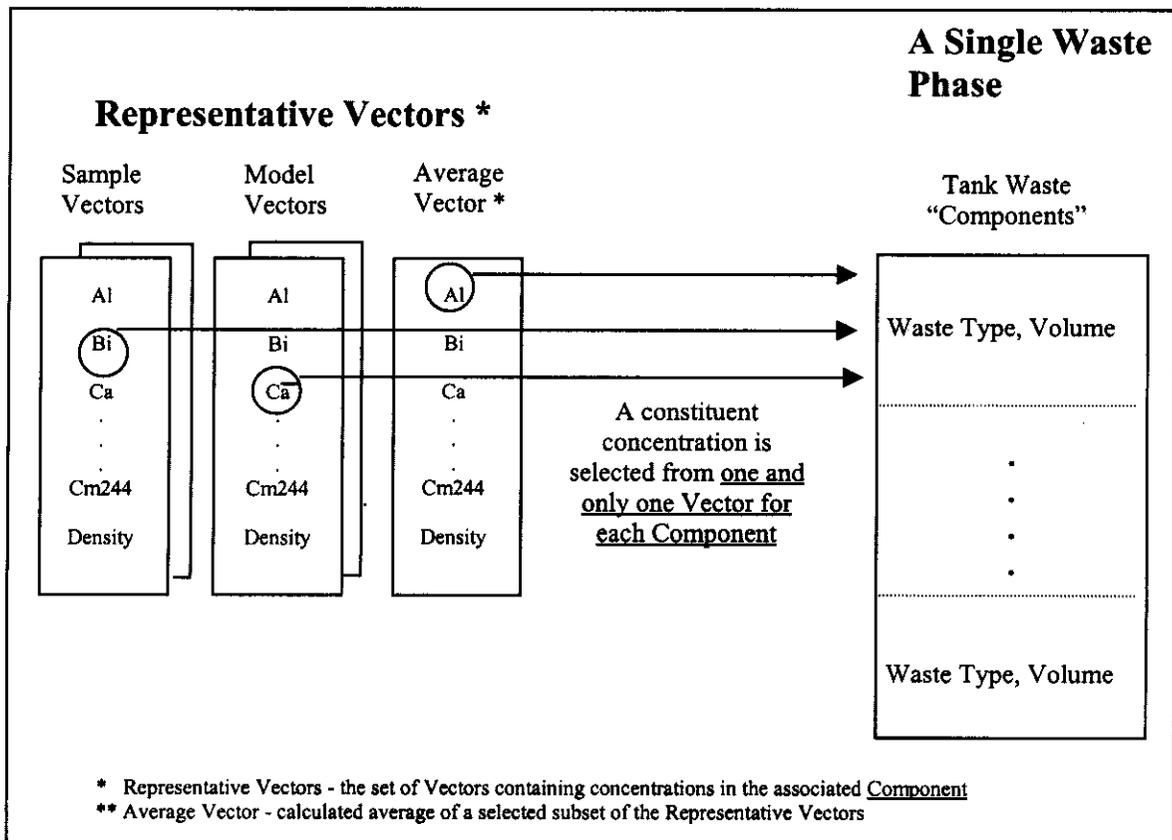
Table 1-1. BBIM System Major Components

Component	Description
BBIM database	SQLServer working database where data are entered and calculated results are reviewed and approved for publication into the public domain. This database contains the database integrity logic, and the best-basis calculations and dependency logic. BBIMCOMBO is the primary user interface for entering data into this database.
BB_Published database	SQLServer database where the BBIM inventories and other subsets of the BBIM database needed for reporting are stored when a tank is published. CONFIGMGNT is the primary user interface for entering data into this database.
BBIMCOMBO	Microsoft Access user interface used by best-basis data configuration engineers to enter input data, check calculated results, review data, and produce reports in the BBIM database. Note: CCB_USER is a special limited-access read-only user of this database.
CONFIGMGNT	Microsoft Access user interface used by best-basis data stewards to review the working data in the BBIM database, compare it to published data, and control, document, and record the publication of data to the BB_Published database.

2.0 PHYSICAL WASTE MODEL: HOW THE DATABASE REFLECTS THE PHYSICAL WASTE

The BBIM relational database structure was designed to represent the structure of the tank waste. This was done to provide the best ability to describe tank waste, and to develop meaningful queries and reports in support of tank waste analysis and tank farm operations. The following paragraphs explain some of the fundamental structures and concepts in the BBIM. Figure 2-1 depicts the structures and relationships defined in the following paragraphs of this section. In this figure, where the term "Average Vector" is used, the Best-Basis Inventory community should not interpret it as being equivalent to the term "Template" as commonly understood. Instead, just think of it as a capability of the BBI Tool to dynamically calculate averages based on several referenced source vectors; whenever the source vector is changed, the Average Vector automatically changes.

Figure 2-1. Physical Waste Representation in BBIM



2.1 VECTORS

One purpose of the BBIM Tool is to document the origin of the fundamental parameters that were used to derive the inventories. Two of these parameters – concentration and density – are stored in a BBIM structure called a **Vector**. Each **Vector** is a set of analytes and their associated concentration values; typically taken from a specific column of a table in a document or compiled and submitted as a spreadsheet.

Each vector also contains a value that defines the overall waste density that applies.

Simply stated, a vector contains a set of concentrations for named analytes, and all of the associated metadata, (including density), which documents the data for reference purposes.

Note: Metadata is “data about the data” (i.e., it is contextual information required to interpret the basic data value: 12 ug/g of Aluminum is the basic data, but *where* the sample was taken from, *when* it was taken, how it was *analyzed*, and what *document* it appeared in are all examples of metadata associated with that basic data value.

Vectors can be one of four types:

- Sample - The concentrations are strictly based on laboratory samples
- HDW - The concentrations are obtained from the *Hanford Tank Chemical And Radionuclide Inventories: HDW Model Rev. 4* (Agnew et al. 1997)
- Process Knowledge - The concentrations are based on historical knowledge of the processes that produced the waste
- Sample Average - This is a virtual vector; it does not physically exist in the database; it is computed as an average of several other actual vectors.

A vector often applies to some portion of the total waste in a tank, not necessarily to the totality of the waste. In the BBIM database structure, the specific volume of waste that is represented by a Vector or Vectors is called a **Component** (see Figure 2-1). Vector Data can be reviewed by means of the Vector Data window shown in Figure 2-2.

Figure 2-2. Sample Vector Report

Vector Data						
Vector_Type	Sample	Handle	S/BX107/01	Analysis date	1/1/94	
Template	IC/CW (1)		Ref_Document	BX-108 BB doc		
Waste_Type_ID	241-BX-107		Ref_Table_Name	Compositions of IC/CW Sludges		
Vector_Name	BX-107 IC/CW Sludge		Ref_Table_No	C3-1	Ref_Table_Col	2
Density	1.44					
Constituent Name	Qualifier	Reported Concentration	Units	Standard Concentration	Units	User Comment
Ag	<	0.942	ug/g	0.942	ug/g	
Al		14300	ug/g	14300	ug/g	
Bi		22300	ug/g	22300	ug/g	
Ca		306	ug/g	306	ug/g	
Cd		2.27	ug/g	2.27	ug/g	
Cl		1140	ug/g	1140	ug/g	
Cr		988	ug/g	988	ug/g	
F		9190	ug/g	9190	ug/g	
Fe		11100	ug/g	11100	ug/g	
Hg		0.686	ug/g	0.686	ug/g	
K		283	ug/g	283	ug/g	
La	<	1.61	ug/g	1.61	ug/g	
Mn		84.6	ug/g	84.6	ug/g	
Na		102000	ug/g	102000	ug/g	
Ni		12.2	ug/g	12.2	ug/g	
NO2		12300	ug/g	12300	ug/g	
NO3		137000	ug/g	137000	ug/g	
Friday, October 29, 1999						
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2.2 COMPONENTS

The BBIM uses the term **Component** to refer to a specific volume of a given Waste Type (SMMS1, R1, etc.) believed to exist within a Waste Phase (Sludge, Saltcake, etc.). In other words, a Component is a distinct portion of waste within a tank for which we have a Vector or Vectors describing the chemicals/radiochemicals and their respective concentrations. Thus, a Component within a given tank is a unique combination of Waste Phase and Waste Type with an associated Volume of the waste. All fundamental parameters required to calculate waste inventories are contained in the Vector (analyte concentration and waste density) and the Component (waste volume). The remaining question is, how are specific Vectors associated with Components in order to allow the calculations to occur? The answer lies in the **Representative Vectors** structure.

2.3 REPRESENTATIVE VECTORS

One or more Vectors define the chemical and/or radiochemical makeup of each Component. Vectors contain the best estimates of concentrations of constituents within a Component of tank waste. The set of Vectors assigned to any Component is known as that Component's Representative Vector set.

Vectors can be of four types: Sample, Model, Average (calculated), or Process Knowledge Vectors. Sample Vectors contain concentrations based on an expert's assessment of available laboratory data. Model Vectors contain HDW Rev. 4 (Agnew et al. 1997) concentrations. Average Vectors contain the average concentration values from a specified subset of any Component's Representative Vectors. Process Knowledge Vectors contain concentrations that are inferred by expert judgment and calculations based on an understanding of the processes that produced the waste and can include results of waste transfer/mixing calculations, templates, original data, and heat load calculations.

Finally, a given constituent for a Component can be selected from one and only one Vector within the Representative Vector set. For example, in Figure 2-1, concentrations for aluminum were available from three Vectors. The concentration chosen to represent aluminum in the Component was taken from the Average Vector.

Having now read about these fundamental database structures, please review Figure 2-1 in order to strengthen your understanding of how these BBIM structures, Vectors, Components, and Representative Vectors, work together. This is really the foundation of the BBIM tool, and for the user who wants to understand how the system works, an understanding of this material is essential.

3.0 HOW THE INVENTORY IS CALCULATED

In the BBIM, inventories are either calculated by the “standard” method, or “special” calculations are used. Standard calculations result in inventory values having either an ‘S’ (Sample), an ‘E’ (Engineering Evaluation), or an ‘M’ (Model) Inventory Basis. Section 3.1 describes these standard calculation protocols. Special calculations result in a ‘C’ (Calculated) Inventory Basis. These are described in section 3.2.

Figure 3-1 contains a view of the Best Basis Inventory Calculation Detail Report (further described in Section 5). This report shows the Best-Basis Inventory with a breakdown by waste component with associated basis and calculation formulae. The names in the formulae are described in this section.

3.1 STANDARD INVENTORY CALCULATIONS (S, E, AND M BASES)

Given the preceding discussion, the inventory of a constituent, C, at the Component level is calculated by the BBIM using the basic formulas:

$$\text{Inventory}(C) = \text{Conc}(C) * \text{Rho} * \text{Vol} * \text{Mult} * \text{UnitAdj} \quad [\text{solid units of concentration}]$$

$$\text{Inventory}(C) = \text{Conc}(C) * \text{Vol} * \text{Mult} * \text{UnitAdj} \quad [\text{liquid units of concentration}]$$

$$\text{Inventory}(C) = \text{Conc}(C) * \text{MW}(C) * \text{Vol} * \text{Mult} * \text{UnitAdj} \quad [\text{molar units of concentration}]$$

<i>Rho</i>	=	the density of the Vector in grams per milliliter
<i>Vol</i>	=	the volume of the waste Component
<i>Conc</i>	=	the constituent concentration in that waste component
<i>UnitAdj</i>	=	Adjustment factor to compensate for unit conversions (e.g., .001 Kg/g)
<i>Mult</i>	=	Multiplier – typically equals 1
<i>MW</i>	=	the molecular weight of the constituent

Rho is a Greek letter that commonly denotes a density variable. When the BBIM tool spells out the formulas used to compute analytic inventories, **Rho** denotes density. Standard units of grams/milliliter are implied. The BBIM records the value of **Rho** every time a new vector is created. If vectors are averaged, **Rho** is averaged.

Mult is the abbreviation used on several reports to denote a multiplier. The multiplier is commonly used to adjust all concentrations within a vector to account for the modification of a specific parameter such as volume, density, or wt % water. It is also used for wt% water, density or concentration adjustments where sample data differs from template/HDW model assumptions.

Component inventories within a single Waste Phase are added to obtain the Total tank inventory for each constituent. Similarly, the BBIM determines the Basis for each Component and for the Total tank inventory based upon the type of Vectors that were selected to calculate the inventory. If all Vectors were Sample, the Total inventory Basis would be "S". If all Vectors were Process Knowledge, the Total inventory Basis would be "E". If all Vectors selected were HDW vectors, the Total inventory Basis would be "M". If a combination of Vector types is used, the Total inventory Basis reflects all types. For example, "S/E" would indicate that one or more Components were S-based, and one or more were E-based. Any combination of "S", "E", and "M" can exist.

Figure 3-1. Simple Calculation Details

Best-Basis Inventory Calculation Detail Report				
Waste_Site_ID		241-AN-104		
Constituent	Inventory	Basis	Formula	Calculation
Phase/Type:				
AI	1.41E+05 kg	S		
Slurry/SMMA2 (DSSF)	5.30E+04 kg	S	$Rho^{*}Vol^{*}Conc^{*}UnitAdj^{*}Mult$	$1.59 \text{ g/ml} * 1593.86 \text{ kL} * 20900 \text{ ug/g} * 0.001 * 1$
Supernatant/SMMA2 (DSSF)	8.78E+04 kg	S	$Rho^{*}Vol^{*}Conc^{*}UnitAdj^{*}Mult$	$1.4 \text{ g/ml} * 2275.03 \text{ kL} * 27571.4 \text{ ug/g} * 0.001 * 1$
BI	9.96E+01 kg	S/E		
Slurry/SMMA2 (DSSF)	9.96E+01 kg	S	$Rho^{*}Vol^{*}Conc^{*}UnitAdj^{*}Mult$	$1.57 \text{ g/ml} * 1593.86 \text{ kL} * 39.8 \text{ ug/g} * 0.001 * 1$
Supernatant/SMMA2 (DSSF)	0.00E+00 kg	E	$Rho^{*}Vol^{*}Conc^{*}UnitAdj^{*}Mult$	$1 \text{ g/ml} * 2275.03 \text{ kL} * 0 \text{ ug/g} * 0.001 * 1$

3.1.1 Special Treatment of Total Waste Phase

Normally, all Components from all Non-Total Waste Phases are summed to arrive at the total tank inventory. However, the Total Waste Phase is used whenever the best available Representative Vectors contain concentrations representing the total tank composite waste, rather than individual Waste Phases. If a constituent is picked from any Vector assigned to the Total Waste Phase, it removes all other Component inventories for that same constituent. If a constituent is picked from any vector assigned to a Non-Total Waste Phase, it removes the Total Waste Phase Component inventory for that same constituent. In other words, the last selection chosen overrides previous choices. There can be any number of non-Total Waste Phase Components for a given constituent, but only one Total Waste Phase.

3.1.2 Treatment of Density

For S-based Component inventories, the density (Rho) used is the density measured in the laboratory (i.e., it is associated with the specific Sample Vector).

For E-based Component inventories, the density (AvgRho) often used is the average density of the Sample Vectors used to calculate the average concentration (i.e., it is the average of all Sample Vector densities used to calculate the E-based Component concentrations; if any of the Component Sample Vectors has an unknown density, that

Vector does not contribute to the average density calculation). Other sources for the E-based density can be specified, including sample results or those derived from waste transfer calculations.

For M-based Component inventories, the HDW Rev. 4 density (Rho) is used.

3.1.3 Vector Multipliers

For sample-based inventories, the Multiplier, "Mult", is a straight multiplier used to adjust a Vector's concentration to account for some specific factor. For example, the reported concentration may be on a dry weight basis, and the factor would adjust the concentration to account for the presence of water as documented in the laboratory report.

For engineering assessment-based (E) inventories, the Multiplier, "AvgMult" is the simple average of the Multipliers of the Vectors upon which the Average Vector is based.

3.1.4 Average Vectors

Averaging together two or more other vectors creates an **average vector**. Typically an average vector is created when several sample vectors exist for the same waste component, and it is desirable to average their values together to get the best estimate possible.

The Calculation Detail Report in Figure 3-2 shows the formula for average vectors in a slightly different format.

Figure 3-2. Inventory Formula for an Average Vector

Tank Name	Analyte	Waste Phase/Type	Inventory	Inventory Unit	Basis/Inventory Formula	Inventory Calculation
241-A-102	Al	Total	7.02E+03	kg	S	
241-A-102	Al	Total/Aggregate of Tank Wastes	7.02E+03	kg	S	$AvgRho * Vol * AVG(Conc * Mult) / 1000$

The *Inventory Formula* is:

$$AvgRho * Vol * AVG(Conc * Mult) / 1000$$

AvgRho = average density of vectors specified for averaging

AVG(Conc*Mult) = average of the concentration times the respective vector multiplier, for that constituent, for each vector that was used to create the Average Vector. Note that if a concentration is recorded as "NR" (Not Recorded), it is not included in that average calculation of the concentration. For example, assume two vectors are used in the average vector calculations. Vector A has a density of 1.4 and its Al concentration is 100. Vector B has a density of 1.2 and its

Al is "NR". The Average Vector will then have a density of $(1.4 + 1.2)/2 = 1.3$ and an Al concentration of $100/1 = 100$.

In the example shown above, vectors were averaged to generate a value for an Aggregate of Tank Wastes, but this does not have to be the case. Vectors can be averaged for a particular waste component.

In some of the reports you will see the term *AvgMult*. As described in section 3.1.5, this term denotes the average value of the multipliers for an average vector, just as *AvgRho* denotes average density.

3.1.5 Radionuclide Decay Adjustments

All radionuclide inventories are automatically decayed by the BBIM database to a certain "standard" date, currently Jan 1, 1994. Decay logic performs first and second order decays. First-order decay constitutes a loss of material due to decay of the given isotope into daughter isotopes; second-order decay constitutes a gain of the given isotope due to parent isotopes decaying into the given isotope.

3.2 SPECIAL INVENTORY CALCULATIONS (C BASIS)

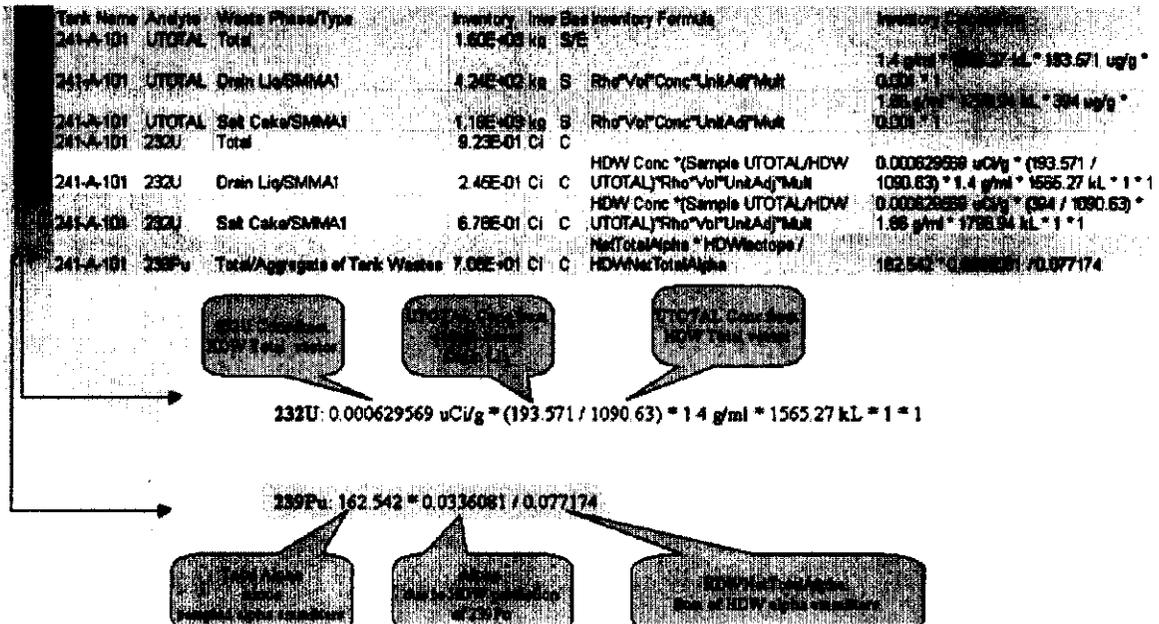
When direct measurements are not available, the inventories of certain analytes can be calculated from more commonly measured analytes based upon known chemical or radiological relationships. The calculations range from simple ratios to charge balances and more complicated isotope ratios (see Figure 3-3). The following sub-sections describe these calculations and how they are applied in the BBIM. The inventories obtained from these calculations have the "C" (Calculated) Inventory Basis.

3.2.1 Simple Ratio Calculations

Certain analytes (typically radionuclides) occur in direct proportion or constant ratios to other analytes. Therefore, by simply multiplying the inventory or concentration of one analyte by a Ratio Factor, the inventory or concentration of another analyte can be determined. Simple ratio inventory calculations take the form:

$$\text{Unknown Constituent} = \text{Known Constituent} * \text{Ratio Factor}$$

Figure 3-3. Special Calculations: Isotopic Distributions Using HDW Rev. 4 Isotopic Ratios



The BBIM currently uses the following simple ratio calculations:

$$\begin{aligned}
 {}^{90}\text{Y} &= {}^{90}\text{Sr} * 1 \\
 {}^{137m}\text{Ba} &= {}^{137}\text{Cs} * 0.946 \\
 {}^{243}\text{Cm} &= {}^{243/244}\text{Cm} * 0.04 \\
 {}^{244}\text{Cm} &= {}^{243/244}\text{Cm} * 0.96
 \end{aligned}$$

Figure 3-4. Detailed Calculations for Barium and Cesium

Isotope	Inventory	Inv Bas	Inventory Formula	Inventory Calculation
137Cs	2.68E+06 Ci	S		
Slurry/SMMA2 (DSSF)	9.60E+06 Ci	S	Rho*Vol*Conc*UnitAdj*Mult	1.67 g/ml * 1693.00 kL * 383.164 uCi/g * 1 * 1
Supernatant/SMMA2 (DSSF)	1.73E+06 Ci	S	Rho*Vol*Conc*UnitAdj*Mult	1.41 g/ml * 2276.03 kL * 638.102 uCi/g * 1 * 1
137mBa	2.54E+06 Ci	C		
Slurry/SMMA2 (DSSF)	9.07E+06 Ci	C	Inventory * Factor	137Cs * 0.946
Supernatant/SMMA2 (DSSF)	1.83E+06 Ci	C	Inventory * Factor	137Cs * 0.946

In Figure 3-4, the basis for 137mBa is "C" (calculated). The inventory of 137mBa is calculated from a formula – 0.946 times the inventory of Cs-137. The inventory of Cs-137 is based on data obtained by sample analysis.

A special case of the dependent calculations is estimating Sr (kg) based on ^{90}Sr (Ci). Whenever Sr is computed in this manner from Sr-90, the BBIM database must convert the inventory of Sr-90, which has units of curies, into an inventory number for Sr, which has units of kilograms. The formula for this conversion is as follows:

IF (we have sample based ^{90}Sr , but don't have Sr for a component)

$\text{Sr}(\text{kg}) = 90\text{Sr}(\text{Ci}) * .024436 / (\text{Rho}(\text{vector}) * \text{Vol}(\text{component}))$

$$.024436 = 1/(0.3*136.4*1000)$$

where 136.4 is the specific activity for Sr-90 and 0.3 is an estimate of the ratio of Sr-90 to Sr in the waste processed through B-Plant.

3.2.2 Isotopic Distribution Using Hanford Defined Waste (HDW) Ratios

Estimation of specific isotopes based on the HDW Rev. 4 isotope ratios is performed on a tank-by-tank basis for a specific set of radionuclides. The ability to do this adjustment depends upon having specific data to work from as follows:

^{232}U , ^{233}U , ^{234}U , ^{235}U , ^{236}U and ^{238}U are based on	UTOTAL.
^{238}Pu , ^{240}Pu , ^{241}Pu , and ^{242}Pu are based on	^{239}Pu or total
^{243}Am , ^{242}Cm , ^{243}Cm and ^{244}Cm are based on	^{241}Am or total

Figure 3-5 shows how these calculations can display. Sample-based source data that have been selected in a vector takes precedence over any Model-based isotope that has been selected in a vector. In the example that follows, it is possible to select the sample based UTOTAL and also the model based ^{238}U , ^{239}U , etc, since these are not mutually exclusive in the radio button form – i.e., they are not the same analyte. But the UTOTAL is still sample based. For example, if UTOTAL has been selected from a Sample-based vector for inventory calculation, then all of the above-named uranium isotopes are calculated based on UTOTAL and the HDW ratios. If, for any reason, the uranium isotopes have also been selected from the M-based vector, these isotope inventories are over-ridden by the automatic calculations. This same principle applies to ^{239}Pu and ^{241}Am and their dependent isotopes. Similarly, if a Sample-Average based UTOTAL has been selected, then it over-rides any M-based isotopes that may have been selected.

If sample-based ^{239}Pu , or ^{241}Am are not available, then a less-desirable form of isotopic estimations can be performed. If TotalAlpha exists, it may be used as a last resort to perform isotope estimation. This is done by first subtracting all uranium isotopes and all alpha-emitting sample-, model-, or process knowledge-based values from the gross TotalAlpha for the whole tank. Then, the remaining alpha is assigned to the previously identified isotopes that do not have sample or process knowledge-based data using the HDW Rev. 4 ratios.

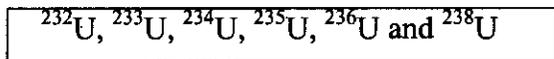
Figure 3-5. Hanford Defined Waste (HDW) Calculations

2UTOTAL	T 5.72E+03 kg	S		
2UTOTAL	T 5.72E+03 kg	S	AvgRho*Vol*AVG(Conc*Mult)/1000	1.645 g/ml * 155.201 kL * 22420 ug/g /1000
2232U	T 3.52E+00 Ci	C	HDW Conc *(Sample UTOTAL/HDW UTOTAL)*Rho*Vol*UnitAdj*Mult	0.000659084 uCi/g * (22420 / 1070.73) * 1.64
2233U	T 1.35E+01 Ci	C		
2233U	T 1.35E+01 Ci	C	HDW Conc *(Sample UTOTAL/HDW UTOTAL)*Rho*Vol*UnitAdj*Mult	0.00252605 uCi/g * (22420 / 1070.73) * 1.645

The following paragraphs describe the HDW Ratioing formulae used for estimating isotopes based on UTOTAL, 239/240Pu, 239Pu, and 241Am. As a last resort, a measurement of Total Alpha is used to estimate alpha-emitting isotopes.

3.2.2.1 Isotopes Based on UTOTAL

Best-Basis uranium isotopes consist of the following:



The formula used to perform the calculation described in the previous paragraph is the following:

$$\text{U-Isotope_Conc} = \text{HDW_Conc} * (\text{Sample_UTOTAL} / \text{HDW_UTOTAL})$$

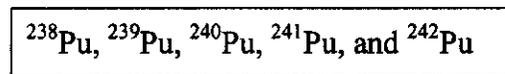
Where:

- U-Isotope_Conc** = **BBIM estimated concentration of U-Isotope**
- HDW_Conc** = **Concentration of U-Isotope estimated by the HDW model**
- Sample_UTOTAL** = **Concentration of Total Uranium per sampling**
- HDW_UTOTAL** = **Estimated concentration of Total Uranium per HDW**

This same technique is used for other isotopes. In each case, an isotope is estimated by taking the amount predicted by the HDW model and multiplying it by a factor. The factor is always computed by measuring the concentration (or amount) of a similar constituent, then by dividing that concentration by the value predicted in HDW.

3.2.2.2 Isotopes Based on ^{239/240}Pu or ²³⁹Pu

The laboratory may in some cases measure ^{239/240}Pu or simply ²³⁹Pu. Either of these measured values can be used in HDW Ratioing to provide estimates for the following isotopes (Pu-241 is actually a beta emitter but it can be estimated by isotopic ratios):



The following formulas are used in these cases:

$$\text{Pu-Isotope_Conc} = \text{HDW_Conc} * (\text{Sample}_{239/240} / (\text{HDW}_{239\text{Pu}} + \text{HDW}_{240\text{Pu}}))$$

$$\text{Pu-Isotope_Conc} = \text{HDW_Conc} * (\text{Sample}_{239} / (\text{HDW}_{239\text{Pu}}))$$

Where:

Pu-Isotope_Conc	=	BBIM Estimated concentration of Pu-Isotope
HDW_Conc	=	Concentration of Pu-Isotope estimated by the HDW model
Sample_239/240	=	Concentration of ^{239/240}Pu per sampling
HDW_²³⁹Pu	=	Estimated concentration of ²³⁹Pu per HDW
HDW_²⁴⁰Pu	=	Estimated concentration of ²⁴⁰Pu per HDW

3.2.2.3 Isotopes Based on ²⁴¹Am

If Am-241 is measured in the laboratory, the following americium and curium isotopes can be estimated:

²⁴³Am, ²⁴²Cm, ²⁴³Cm, and ²⁴⁴Cm

The following formula is used:

$$\text{Am/Cm-Isotope_Conc} = \text{HDW_Conc} * (\text{Sample}_{241} / (\text{HDW}_{241\text{Am}}))$$

Where:

Am/Cm-Isotope_Conc	=	BBIM Estimated concentration of Am/Cm-Isotope
HDW_Conc	=	Concentration of Am/Cm-Isotope estimated by the HDW model
Sample_241	=	Concentration of ²⁴¹Am per sampling
HDW_UTOTAL	=	Estimated concentration of ²⁴¹Am per HDW

3.2.2.4 Isotopes Based on Total Alpha Measurements

If sample-based, ²³⁹Pu or ²⁴¹Am are not available, then a less-desirable form of isotopic estimations can be performed based on Total Alpha data. This technique can be used to estimate the following radionuclides:

²³⁸Pu, ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu, ²⁴²Pu, ²⁴¹Am, ²⁴³Am, ²⁴²Cm, ²⁴³Cm, and ²⁴⁴Cm.

This is done by subtracting uranium alpha, all alpha emitting sample-based values, and those alpha emitters that can be estimated directly from sample-based ²³⁹Pu or ²⁴¹Am from the TotalAlpha for the whole tank. Then, the remaining alpha is assigned to the previously identified alpha-emitting isotopes that do not have sample data and are not

estimated from sample-based ^{239}Pu or ^{241}Am using the HDW Rev. 4 ratios. Plutonium-241 (a beta emitter) can also be estimated from ^{239}Pu using the HDW model Rev. 4 ratios.

Total Alpha factoring works similarly to the other factoring techniques, but the formula is different:

$$\text{Isotope_Conc} = \text{NetTotalAlpha} * \text{HDWIsotope} / \text{HDWNetTotalAlpha}$$

Where:

NetTotalAlpha	=	measured value of Total Alpha minus uranium alpha and any alpha that can be derived from sample-based isotopes that have been selected.
HDWIsotope	=	alpha contribution of the isotope predicted by the HDW model.
HDWNetTotalAlpha	=	sum of HDW predictions of any alpha-emitters included in the NetTotalAlpha (excludes uranium alpha or any alpha emitter than can be derived from the selected sample-based isotopes).

IMPORTANT NOTE

Total Alpha distribution IS ONLY DONE AT THE TANK LEVEL – the algorithm is unable to apply this technique at the waste component level!

3.2.3 Charge Balance Adjustments

At equilibrium, the charge balance equation states that the total quantity of negative charges should equal the total quantity of positive charges. An imbalance may be an indicator changes to the chemical composition of the material under consideration are incomplete. In the Best-Basis Inventories, charge balancing was performed using an algorithm, which calculated the charge contribution for the analytes based on their predicted mass (Best-Basis Inventory). Total hydroxide (OH⁻Total) was not directly entered into the database and valence model, but was determined by difference to achieve a balance between the positive and negative ions. This is done on a tank-by-tank basis so that each tank comprises a charge-neutral chemical system.

The use of hydroxide ion for charge balancing is for convenience. The actual tank waste may contain metal oxides rather than hydroxides. (Especially for sludge layers.)

- Charge balance
- 017007*SUM(Valences*kgs*1000/MWs)
- Can only be done at Publication time because of the requirement to be able to “Lock” previously published constituents that may be anions or cations.

In cases where a net positive charge is calculated for the measured or estimated anions and cations, the BBI Tool will calculate a negative quantity of OH⁻.

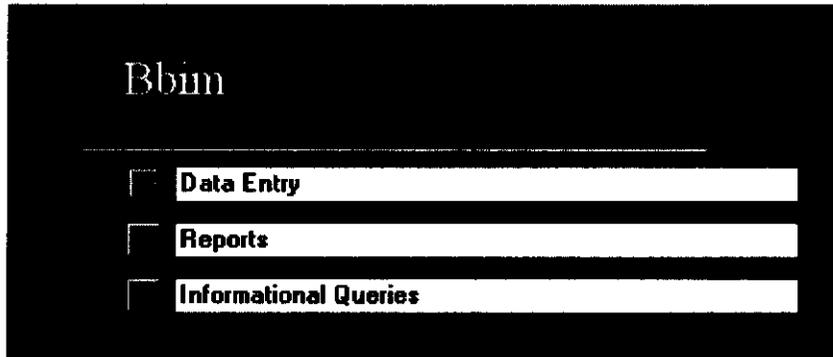
3.3 TOTAL WASTE PHASE

The **Total Waste Phase** is a special phase that applies to the total tank. If a concentration is defined in the *Total Waste Phase*, it “overrides” corresponding values set in the other waste components. When this happens, the inventory for the constituent is taken directly from the *Total Waste Phase*, rather than summing the inventory of the other waste components. *Total Waste Phase* concentrations are identified in the *Waste Phase/Type* column as *Total/Aggregate Waste Phases*, as shown earlier in Figure 3-2.

4.0 THE DATA ENTRY PROCESS (BBIMCOMBO)

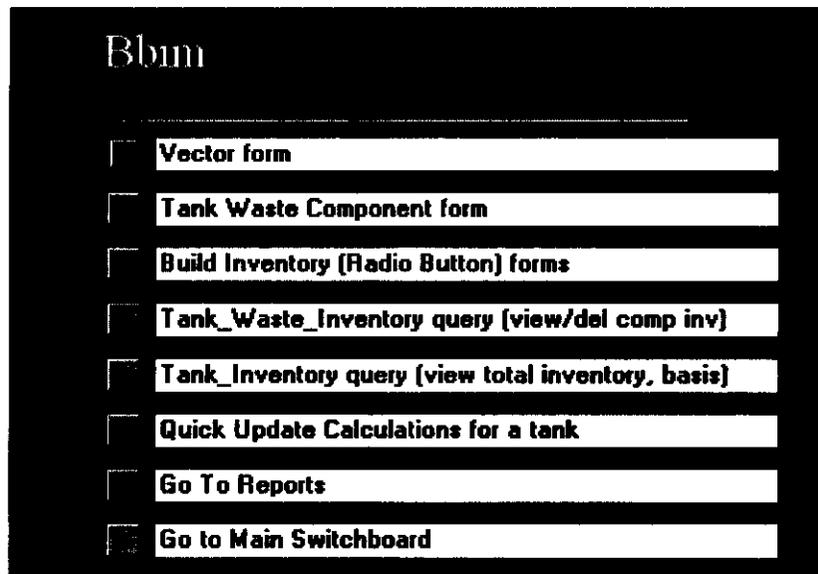
This chapter describes the data entry process and how the best-basis inventory is created and updated. This chapter also explains the data entry portion of BBIMCOMBO, a software program that connects users to the BBIM database application.

Figure 4-1. Main Switchboard



From the Main Switchboard shown in Figure 4-1, the **Data Entry** form is designed to follow the logical sequential steps of BBIM data entry, from the top to the bottom of the form, starting with the **Vector** form (see Figure 4-2).

Figure 4-2. Data Entry Switchboard



4.1 VECTOR FORM

The purpose of the **Vector** form is to allow the creation and update of Vectors. To access the **Vector** form, log onto BBIMCOMBO, select **Data Entry** and then **Vector Form**. The **Vector** form will appear as illustrated in Figure 4-3.

Figure 4-3. Vector Form

Vector_Type	Sample	Sample_Date	Ref_Table_No
Template	SMMS1	Decay_Date_Reported	Ref_Table_Column_No 2
Vector_Waste_Site_ID	241-S-101	Ref_Document	Template file
Vector_Name	Segments 2L-4U	Lock This Vector	
Density	1.58	Ref_Table_Name	SMMS1 Salt Cake Concentrations
Bogus_Density (Y/N)?		Vector_Handle	S/S101/01
Vector Constituents		Density_Comment	
Symbol	Concentration	Units	Comment
Ag	12	ug/g	Units Updated (2)
Al	18000	ug/g	Units Updated (2)
B	110	ug/g	Units Updated (2)
Bi	71	ug/g	Units Updated (2)
Ca	273	ug/g	Units Updated (2)
Cl	4500	ug/g	Units Updated (2)
Cr	10000	ug/g	Units Updated (2)
F	500	ug/g	Units Updated (2)
Fe	508	ug/g	Units Updated (2)
K	1109	ug/g	Units Updated (2)
La	<DL	ug/g	Units Updated (2)

Record 1 of 1

Vector_Type is a required field. It designates whether the data came from:

- Sample Analysis (*Sample*), or
- A Model (*HDW*), or
- Process Knowledge (*Process Knowledge*)

A vector cannot contain mixed data, such as a combination of data from sample analysis and from process knowledge.

A **Template** is a waste type that will be used repeatedly. If a vector is used to construct a template, the template name must be entered in this field. In order to be selected from the pull-down list, the template name should be identified before hand. If the vector will not be used as part of a template, select *N/A*.

Vector_Name is a required field. A vector must be assigned a name (typically, it would be the column name if extracted from a table in a document).

Density is a required field – so that mass concentration can be adjusted to volumetric concentration when required. Standard density units of grams/milliliter are implied. If the density is unknown, an estimated density is entered, and **Bogus_Density** is set to yes. This will flag the density as an estimate, and a more precise value should be entered when available. In the meantime, the density will allow BBIM to use the vector. (The BBIM database insists that density be entered).

Vector Handle is a unique identifier for a vector. It is computed automatically by BBIMCOMBO.

Normally, you will be expected to document where the vector came from and the reported decay date by filling out the following fields:

Sample_Date – when sampling was done (for sampled data only)

Decay_Date_Reported – for radioactive constituents

Ref_Document - name of document

Ref_Table_Name – name of the table from which numbers were taken.

Ref_Table_No – number of the table from which numbers were taken

Reference Table Column Number – column number used from the table

Once the vector and its source document are described, you can identify the constituents and identify the concentrations in the **Vector Constituents** sub-form. The computer updates the **vc_id** column on the sub-form automatically.

4.1.1 Allowable Units of Reported Concentration

The following table shows the allowable concentration units that can be entered into the **Vector** form as Reported Concentration and Units. These are then converted to Standard Concentration (Std_Concentration) with the Standard Units of Concentration (Std_Units) as shown in the table (always ug/g for Chemicals and uCi/g for Radiochemicals). When the calculation of Inventory is done, it uses the Std_Concentration and the Units of Inventory are always Kg for Chemicals and Ci for Radionuclides.

Table 4-1. Conversion of Reported Units of Concentration into Inventory (2 sheets)

Reported Concentration	Standard Concentration	Units of Inventory
M	ug/g	Kg
ug/g	“	“
g/g	“	“
ug/l	“	“
Kgal	“	“
g/mL	“	Kg
mg/L	“	“

Table 4-1. Conversion of Reported Units of Concentration into Inventory (2 sheets)

Reported Units of Concentration	Inventory Units of Concentration	Units of Inventory
ug/mL	ug/g	"
wt%	"	"
wt% C (wet)	"	"
uCi/g	uCi/g	Ci
Ci/mL	"	"
Ci/L	"	"
uCi/L	"	"
mCi/L	"	"
uCi/mL	"	"

4.1.2 Special Conversions at Input Time

The **Vector Constituents** subform performs several special conversions. These are described in the following paragraphs.

4.1.2.1 TIC as CO3

The **Vector** form will accept either "TIC" or "CO3" as input, while immediately converting to a different constituent name, "TIC as CO3". If the input constituent name is TIC, it must be multiplied by a factor of $60/12 = 5$ for conversion. Total Inorganic Carbon, or TIC is measured in the laboratory, but is assumed to exist in the form of CO3 in the waste. Therefore, the concentration must be multiplied by the ratio of the molecular weights. The reported value is maintained in *Comment* field along with a description of the conversion.

4.1.2.2 P as PO4

The **Vector** form will accept either "P" or "PO4" as input, while immediately converting to a different constituent name, "P as PO4". If the input constituent name is P, it must be multiplied by a factor of $95/31$ for conversion. Phosphorous, or P is measured by the ICP analysis method in the laboratory, but is assumed to exist in the form of PO4 in the waste. Therefore, the concentration must be multiplied by the ratio of the molecular weights. However, PO4 can also be directly measured in the laboratory by the IC method. The reported value is maintained in *Comment* field along with a description of the conversion.

4.1.2.3 S as SO4

The **Vector** form will accept either "S" or "SO4" as input, while immediately converting to a different constituent name, "S as SO4". If the input constituent name is S, it must be multiplied by a factor of $96/32$ for conversion. Sulfur, or S is measured in the laboratory, but is assumed to exist in the form of SO4 in the waste. Therefore, the concentration

must be multiplied by the ratio of the molecular weights. However, SO4 can also be directly measured. The reported value is maintained in *Comment* field along with a description of the conversion.

4.2 TANK WASTE COMPONENT FORM

The purpose of the **Tank Waste Component** form (see Figure 4-4) is to allow the creation and update of Components and their alignment with Representative Vectors.

Once vectors describing the concentrations of individual constituents have been created, the Component is then created and the vectors are related to the waste components. These last two functions are performed using the **Tank Waste Component** form shown below. As mentioned previously, a Waste Component is a specific volume of waste in a tank that consists of a single phase of material, which has been identified as having a consistent chemical makeup.

Figure 4-4. Waste Component Form – Subform is left justified

TWT_ID	2		
Waste_Site_ID	241-AN-106	Vol_Reference	
Waste_Phase	Sludge	Input_Data_Location	
Waste_Type	CP		
Volume	64.4		
Units_of_Volume	kL		

After adding a new record in the table below, go to the next or previous record, then back again to view the new record.

Waste_Site_ID	Waste_Phase	Waste_Type	Volume	Units_of_Volume	Vol_Reference	Input_Data_Location
241-AN-106	Sludge	CP	64.4	kL		
241-AN-106	Sludge	CP	64.4	kL		

To access the **Waste Component** form, log onto BBIMCOMBO, select *Data Entry* and then select the *Tank Waste Component Form*.

The first field on the form, *TWT_ID* is filled in by the computer. Ignore this field during data entry.

Each waste component must be assigned a *Waste_Site_ID* (tank name) and a *Waste_Phase*.

Waste_Type is a way of classifying waste. Numerous waste types have been defined at Hanford over the years. A recent system for classifying wastes is the Hanford Defined Waste (Rev. 4) model. This model defines some 40 waste types. Often, when a waste type originally defined within the HDW model is used, the Best-Basis team has assigned a “Template” vector to represent that waste type. The Template vector may have been created by averaging the vectors from several tanks or sampling efforts.

Volume and *Units_of_Volume* are required fields that specify the volume of waste in the component that is being described.

Vol_Reference and *Input_Data_Location* are optional fields that are used to specify any documents associated with the waste component.

Vector Subform

At the bottom of the **Tank Waste Component** form is the **Vector** subform. The purpose of the **Vector** subform of the **Tank Waste Component** form is to link the vector(s) previously created to the current Component.

Initially, this subform will be empty – no records will appear – because initially, no Vectors are linked to the Component you are currently creating. The procedure for identifying a vector is to tab to the *Type, Template, Waste_Site_ID, Vector_Name* field, and select a previously defined vector from the drop-down selection control. Once you have selected a previously created Vector, all of the fields will be filled out with all of the information previously entered when the Vector was created. Congratulations! You have just linked this Vector with this Component!

You can create a new vector through this form, if you wish, although it is not recommended. If so, or if you wish to create an Average Vector, you must fill out several extra fields as described below.

The first field on the sub-form is titled *Tank Waste Component*. This value is derived from three fields on the main form: *Waste_Site_ID, Waste_Phase,* and *Waste_Type*. Do not enter anything in this field. Let the computer fill it in when the record is saved.

Include In Avg is a mandatory field that indicates whether the vector is being used to create an Average Vector. As mentioned previously, an Average Vector is computed by averaging several vectors together (typically sampling data vectors). Normally, you will ignore this field. The default selection is *N* (no). Select *Y* if you wish to include the vector in an Average Vector (for this waste component). All Vector records in this subform that have a ‘Y’ in this field will be averaged together to create an “Average Vector” which is not a physical vector but a “virtual” vector.

Significance is an artifact of previous programs. Ignore it.

Multiplier can be used to scale concentrations within the vector because of special circumstances, as explained previously. Normally you will ignore this field. The default value is 1. If you choose to apply a scalar value other than one, it is strongly recommended that you explain the reason in the *Multiplier Description* column.

Vectors are added to the sub-form by selecting them from the *Type, Template, Waste_Site_ID, and Vector_Name* pull-down lists.

Vector.V_ID is an auto-number field that is filled in and used by the computer. Ignore it.

4.3 BUILD INVENTORY (RADIO BUTTON) FORMS: BUILDING THE WASTE PHASE INVENTORY

After you relate vectors to a waste component, you can build the inventory. A matrix of constituents and vectors is created on a **Radio Button** form. You can select the proper value for each constituent using this form.

IMPORTANT NOTE: The contents of the Radio Button form are not directly linked to the Vectors and Components. What this means is that if you call up the Radio Button form and then call up a Vector form at the same time and modify the Vector, that update will not be reflected in the Radio Button form; you must exit from the Radio Button form and restart it!

Build Form

To access the **Build Inventory** form, log onto BBIMCOMBO, select *Data Entry* and then *Build Inventory (Radio Button) Form*.

The top half of the form shows the *Waste_Site_ID, Waste_Phase, and Waste_Type* -- allowing you to navigate to the Waste Component of interest (see Figure 4-5).

Once you are on the correct record, you may use the *Analytes* block to designate whether you wish to build an inventory for a single constituent or a group of constituents.

On the sub-form, check *Include* for each vector that will be used when describing the inventory. If you created an Average Vector previously, it should show up in this sub-form.

Next, press the **Build Form** button.

Figure 4-5. Radio Button Build Form -- Part 1

Build Inventory Basis Selection Form For:

Waste Site ID: 241-A-101
 Waste Phase: Drain Liq
 Waste Type: SMMA1
 Volume: 1565.267862

Analytes

Group Chemical
 Single

Waste ID	Waste Type	Matrix	Vector Type	Vector Name
<input type="checkbox"/> S/A101/03	SMMA1	NA	Sample	241-A-101 , Drainable Liquid Mean

Radio Button Form

Be patient. It may take BBIMCOMBO a while (on the order of a minute) to build the **Radio Button** form. When the form is ready for viewing, you will see an array of radio buttons, which describe the present inventory calculation basis (see Figure 4-6). Each row corresponds to a different constituent, each column is for a different vector. A black radio button indicates that the vector value was selected for that constituent. A white unselected radio button indicates that the vector value was not selected.

Figure 4-6. Radio Button Form -- Part 2

Form1 Form

Choose Best Basis for Tank: 241-A-102, Waste Phase: Total
 Waste Type: Aggregate of Tank Wastes, Volume: 155.2014 (kL)

View Phase Inventory View Tank Inventory Update Inventory

Constituent	H/A102/01 HDW 241-A-102, Total Inventory Estimate	P/U107/04 Process Knowledge 241-U- 107, Process Knowledge	S/A102/01 Sample 241-A-102 , 1986 Core Composite Analysis	S/A102/02 Sample 241-A-102 , 96-AUG-003 sample	Sample Average (Calculated)
Radio Button	Radio Column	Radio Column	Radio Column	Radio Column	Radio Column
Ag	<input checked="" type="radio"/> NR	<input checked="" type="radio"/> NR	<input checked="" type="radio"/> 247 ug/g	<input checked="" type="radio"/> 371 ug/g	<input checked="" type="radio"/> 309 ug/g
AJ	<input type="radio"/> 1.43364 M	<input type="radio"/> NR	<input type="radio"/> 2.33E+04 ug/g	<input type="radio"/> 3.17E+04 ug/g	<input type="radio"/> 2.75E+04 ug/g
B	<input checked="" type="radio"/> NR	<input checked="" type="radio"/> NR	<input checked="" type="radio"/> 14.2 ug/g	<input checked="" type="radio"/> < 52.3 ug/g	<input checked="" type="radio"/> 33.25 ug/g
Ba	<input checked="" type="radio"/> NR	<input checked="" type="radio"/> NR	<input checked="" type="radio"/> 880 ug/g	<input checked="" type="radio"/> 139 ug/g	<input checked="" type="radio"/> 509.5 ug/g
Bi	<input type="radio"/> 1.04056 M	<input type="radio"/> 0.00E+00 ug/mL	<input type="radio"/> 1740 ug/g	<input type="radio"/> 336 ug/g	<input type="radio"/> 1038 ug/g
Ca	<input type="radio"/> .033265 M	<input type="radio"/> 0.00E+00 ug/mL	<input type="radio"/> 2590 ug/g	<input type="radio"/> 690 ug/g	<input type="radio"/> 1640 ug/g
Cd	<input checked="" type="radio"/> NR	<input checked="" type="radio"/> NR	<input checked="" type="radio"/> 64.9 ug/g	<input checked="" type="radio"/> 76.5 ug/g	<input checked="" type="radio"/> 70.7 ug/g

You may view a report that shows the present inventory settings for the waste component. The report can show the inventory for each Waste Phase/Waste Type (i.e., for each Component), or across the entire tank. To see these reports, press *View Phase/Type Inventory*, or press *View Tank Inventory*.

To change the concentration of a constituent, click on a radio button belonging to that constituent, which has the value you wish to select.

Important:

After your selections have been made, you must press *Update Inventory* to finalize the changes, otherwise the existing inventory will remain in effect and your changes will be lost.

4.4 TANK_WASTE_INVENTORY QUERY (VIEW/DEL COMP INV)

After the inventories have been initially built, some tools are needed to maintain them. This query is one of those tools.

This query returns a record for each constituent inventory in the Tank/Waste_Phase/Waste_Type specified. This is useful for viewing the details surrounding the inventory, *but mostly this query is useful for deleting all or part of the Component-level inventories*. Deletion of a single inventory record is accomplished by selecting the record by clicking on the left-most part and hitting the **Delete** key. Multiple records can be selected with shift-click or Ctrl-click, or the entire set of records can be selected by clicking in the upper left most portion of the grid.

4.5 TANK_INVENTORY QUERY (VIEW TOTAL INVENTORY, BASIS)

This query returns a record for each total inventory value for a specified tank, along with the Inventory Basis, which is a composite of the Component Bases. The total tank inventory is automatically updated whenever you update a tank's Component inventory by clicking **Update Inventory** from the **Radio Button** form, or by doing a **Quick Update**.

4.6 QUICK UPDATE CALCULATIONS FOR A TANK

You may wish to update tank inventories without going through the **Radio Button** form. For example, you may want to modify existing vector values that are already associated with a waste component. To do so, access the **Data Entry** form and press the button for **Quick Update Calculations for a tank**. Navigate to the tank and waste phase you wish to update. You may update all the waste phases for a tank at one time by checking the **All Waste Phases** box. Press the **Update Now** button, and the computer will update the inventory for you.

5.0 REPORTS AND QUERIES (BBIMCOMBO)

5.1 REPORTS

On selecting *Reports* from the main Switchboard, the **Reports Switchboard** form shown in Figure 5-1 is displayed:

Figure 5-1. Reports Switchboard

Checkbox	Report Name
<input type="checkbox"/>	Calculation Detail report
<input type="checkbox"/>	Tom's Comparison Report
<input type="checkbox"/>	Summary report
<input checked="" type="checkbox"/>	Representative Vector report
<input checked="" type="checkbox"/>	Vector report
<input type="checkbox"/>	Radio Button report
<input type="checkbox"/>	Template report
<input type="checkbox"/>	View Pending Inventory Changes report
<input checked="" type="checkbox"/>	Pre Publication OH report
<input checked="" type="checkbox"/>	Go to Main Switchboard

These reports are described in Table 5-1. Note the column, "CCB_USER". This column identifies the BBIMCOMBO reports that are available in the limited-access read-only version of BBIMCOMBO that is provided to users who log in as "ccb_user". A 'Y' indicates the item is available to CCB_USER.

Table 5-1. BBIMCOMBO Reports (4 sheets)

Report Name	Report Description	Query Parameters	CCB_USER
		Note: where the character, "*" is mentioned in this column, it refers to a "wildcard character" which matches any character string. Thus, *AX* matches all of the AX farm tanks.	
Calculation Detail Report	Provides the inventory, basis, formula, and calculation by waste phase/type for each analyte.	Enter tank name (241-XX-YYY) or * for all tanks and click OK. Next enter the constituent name or * for all constituents and click OK. The constituent is the chemical symbol corresponding to the BBI standard analyte or other analytes used to derive BBI standard analyte inventory values (e.g., ^{239/240} Pu, total alpha, ^{243/244} Cm, etc.). Type the radionuclide constituents with atomic number first (e.g., ⁹⁰ Sr, ¹³⁷ Cs, etc.).	Y

Table 5-1. BBIMCOMBO Reports (4 sheets)

Report Name	Report Description	Query Parameters	CCB USER
Tom's Comparison Report	This report shows the published inventory value, basis, and comment (accessible via the TWINS interface) and the BBIM inventory value, basis, and comment (contained in the BBIM Tool). It also defines the relative percent difference (RPD) between the two inventory values. The update mode is also shown for each analyte, along with a justification for either locking on the published value or forcing the BBIM value to overwrite the published value. In instances where the RPD between the published and BBIM values is $<+1\%$, no update mode or justification is required for the BBIM value to overwrite the published value (at the time the BBIM work unit is published).	Highlight a tank from the dropdown list and then hit the View Tank CM Report button. If the tank you are looking for is not in the dropdown list, it is because the tank inventory has already been published via the BBIM Tool for viewing in TWINS. Once publication has occurred, a comparison between the published inventory value and the BBIM value is no longer valid.	Y
Summary Report	Provides an overview of which concentration vectors and volume are associated with each waste phase/type.	Enter tank name (241-XX-YYY) or * for all tanks.	Y

Table 5-1. BBIMCOMBO Reports (4 sheets)

Report Name	Report Description	Query Parameters	CCB_USER
Representative Vector Report	Provides the meta data and concentration values for each vector associated with a tank inventory and that meet the vector-type search criteria (H*, S*, P*, or *). The values in the reported concentration column correspond to source data and the values in the standard concentration column are the source values reported in standard units (ug/g or uCi/g and decayed to 1/1/94). The analysis date at the top of each vector report is used as the basis for decay.	Enter vector type as H* (HDW vectors only), P* (process knowledge vectors only), S* (sample vectors only), or * (all vector types). Next, enter tank name (241-XX-YYY) or * for all tanks.	Y
Vector Report	Provides the meta data and concentration values for a specified vector or vectors meeting the search criteria. The values in the reported concentration column correspond to source data and the values in the standard concentration column are the source values reported in standard units (ug/g or uCi/g and decayed to 1/1/94).	Enter Vector Tank Name or * for all tanks. Next, enter vector type as H* (HDW vectors only), P* (process knowledge vectors only), S* (sample vectors only), or * (all vector types). Next, enter the vector handle (e.g., S/AN102/01, H/AP102/*, etc.) or * to get all vectors.	
Radio Button Report	This report identifies which concentration value was selected by analyte by waste phase/type to generate the analyte inventory. The concentration values are in "reported" not standard units.	Highlight a tank from the dropdown list and then hit the Assemble Report button.	Y

Table 5-1. BBIMCOMBO Reports (4 sheets)

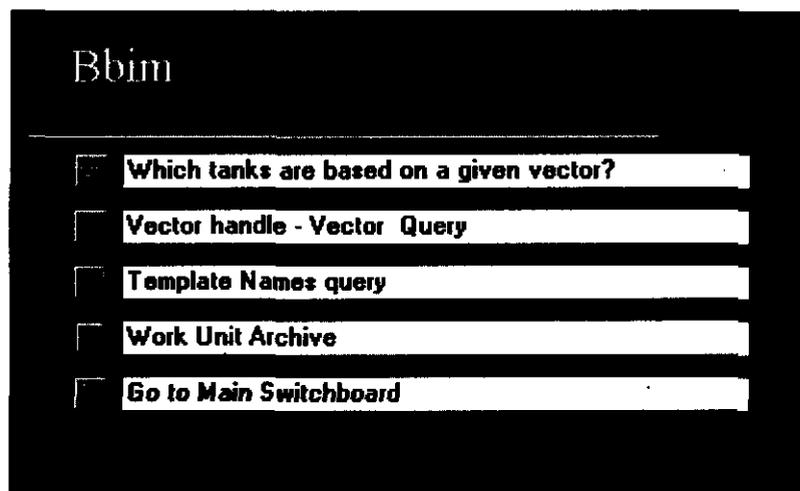
Report Name	Report Description	Query Parameters	CCB USER
Template Report	Provides a vector report for all vectors used to derive the selected template. The report is in a similar form to the Representative Vector Report; however, no vector handles are included, no analysis date is provided, both concentration values shown are in standard units, and only BBI standard analytes are listed (e.g., ^{239/240} Pu will not appear on this report).	Enter template name as defined in the Template Names query under Informational Queries (e.g., CWR1, SMMA1, T1StCk, etc.).	Y
View Pending Inventory Changes Report/Fixed Inventory Record	<p>Provides both the published inventory value (the inventory value available via TWINS and reported in the current column of this report) and the BBIM inventory value (in the pending column of this report) by analyte. In addition, the update mode, RPD between the two values, the comment to be published, and the associated change log number are shown in this report.</p> <p>Once you close out of the View Pending Inventory Changes Report, the Fixed Inventory Record will appear showing inventory values with RPDs exceeding $<\pm 1\%$ that have not been either locked or forced.</p>	Highlight a tank from the dropdown list and then hit the View Pending Inventory Changes button. If the tank you are looking for is not in the dropdown list, it is because the tank inventory has already been published via the BBIM Tool for viewing in TWINS.	Y

Table 5-1. BBIMCOMBO Reports (4 sheets)

Report Name	Report Description	Query Parameters	CCB_USER
Pre-Publication OH report	Shows the calculated values of OH that would be created in the BB_Published database if the specified tank were to be published at the current time. Note: OH can only be calculated at Publish time and not prior because the knowledge of which inventory values are "Locked" and "Forced" are only set at Publish time. The purpose of this report is to provide the ability to verify the OH calculations prior to putting them into the public domain.	Highlight one of the tanks from the list box. If the tank you are looking for is not in the dropdown list, it is because the tank inventory has already been published via the BBIM Tool for viewing in TWINS.	

5.2 INFORMATIONAL QUERIES

On selecting *Informational Queries* from the main Switchboard, the **Informational Queries Switchboard** form, shown in Figure 5-2, is displayed:

Figure 5-2. Informational Queries Switchboard

These Informational Queries are described in Table 5-2.

Table 5-2. BBIMCOMBO Informational Queries

Query Name	Query Description	Query Parameters
Which tanks are based on a given vector?	If you know the concentration vector handle or the approximate vector name (use a * for a wild card), then this report will identify the tanks having inventory values dependent on this vector. The query results will also include tanks to which the selected vector is linked but never actually selected from to derive an inventory value.	Enter the vector handle (e.g., S/AN102/01, H/AP102/*, etc.) and then enter the vector name if known, otherwise enter *.
Vector Handle - Vector Query	Provides a list of all concentration data and associated meta data meeting the query criteria.	Enter the vector handle (e.g., S/AN102/01, H/AP102/*, etc.) or * to get all vectors. Next enter the vector name or *.
Template Names Query	Lists all the template names contained in the BBIM Tool.	N/A
Work Unit Archive	Historical record of activities associated with work units. See Figure 5-3 for more details.	Enter Work Unit, Name of person who updated, CCB Log #, State, Earliest Date.

Figure 5-3. Work Unit Archive Informational Query

Status	Date/Time	CCB	Activity	Description	Tank	Work Unit
Pending	12/1/99 11:09:36 AM prindville	CCB-081	Revised TCR	Revised New sample based inventory	Single Tank	241-U-105
Pending	12/1/99 11:09:29 AM prindville	CCB-087	Revised TCR	Revised Saltwell Pumping and new waste t	Single Tank	241-T-110
Pending	12/2/99 11:15:42 AM prindville	CCB-076-003	Waste Transfer Update	Revised Inventories must be modified to ac	Single Tank	241-AP-107
Pending	12/3/99 8:56:27 AM prindville	CCB-087	Revised TCR	Revised Saltwell Pumping and new waste t	Single Tank	241-T-110
Pending	12/2/99 3:55:21 PM prindville	CCB-076-003	Waste Transfer Update	Revised Inventories must be modified to ac	Single Tank	241-AP-107
Pending	12/2/99 1:09:56 PM prindville	CCB-076-016	Waste Transfer Update	Revised Inventories must be modified to ac	Single Tank	241-SY-102
Pending	12/3/99 2:22:59 PM prindville	CCB-070-108a	Codification Phase II	Revised Correct mathematical, decay, and	Single Tank	241-T-101
Pending	12/6/99 10:25:01 AM prindville	CCB-087a	Revised TCR	Revised Saltwell Pumping and new waste t	Single Tank	241-T-110
Pending	12/2/99 3:55:36 PM prindville	CCB-085	Revised TCR	Revised Inventories must be modified to ac	Double Tank	241-AP-106
Pending	12/8/99 7:30:39 AM prindville	CCB-085	Revised TCR	Revised Inventories must be modified to ac	Double Tank	241-AP-106
Pending	12/1/99 12:56:31 PM prindville	CCB-081	Revised TCR	Revised New sample based inventory	Single Tank	241-U-105
Pending	12/1/99 1:33:14 PM prindville	CCB-084	Revised TCR	Revised New sample based inventory	Single Tank	241-U-103
Pending	12/8/99 3:32:59 PM prindville	CCB-081	Revised TCR	Revised New sample based inventory	Single Tank	241-U-105
Pending	12/8/99 3:39:21 PM prindville	CCB-084	Revised TCR	Revised New sample based inventory	Single Tank	241-U-103
Pending	12/8/99 2:01:00 PM prindville	CCB-091	Revised TCR	Revised Saltwell Pumping and new waste t	Single Tank	241-T-104
Pending	12/7/99 10:45:56 AM prindville	CCB-089	Revised TCR	Revised Saltwell Pumping and new sample	Single Tank	241-AP-103

5.3 TWINS BEST-BASIS REPORTS

TWINS can be accessed on the INTERNET at <http://twins.pnl.gov/twins3>.

To access the BBIM database reports from the TWINS web page, click on the desk calculator that says *DATA*. A new form will appear that is titled Tank Waste Information Network System. Click on the hyperlink that says *Data Source Selection Forms*. The computer will pause for a few seconds and then should provide a menu of subject areas. Select *Best Basis Inventory*. Several report options are available.

Calculation Detail

Shows the details of the calculations used to compute the inventory for each tank/waste phase/constituent combination.

Summary Report

Shows the total tank inventory for each constituent for each tank.

TCR Tank Inventory

Shows the bulk (total) inventory for each tank. It also shows the date each inventory number was computed, the date published, and the associated documentation and change request numbers.

Change Control Status

Shows the proposed and/or approved changes.

TWRS Planning Baseline as of date mm/dd/yyyy

Shows the total tank inventory for each constituent, for each tank, at the time of the baseline date.

Uncertainty Estimates

This report is not part of the BBIM database. Uncertainty estimates are presented as probability distributions, which are quantified as percentiles. Each row presents the probability distribution estimate for a given constituent in a stated tank. See User's Guide for Best-Basis Standard Inventory Uncertainty Estimation Results in TWINS/TCD for more information.

Wash and Leach Factors

This report is not part of the BBIM database. The data in the report are intended specifically as input data for the Hanford Tank Waste Operations Simulator (HTWOS). The data may be utilized for other purposes, but the user has the responsibility of ascertaining that the use of these simplified wash and leach factors is appropriate.

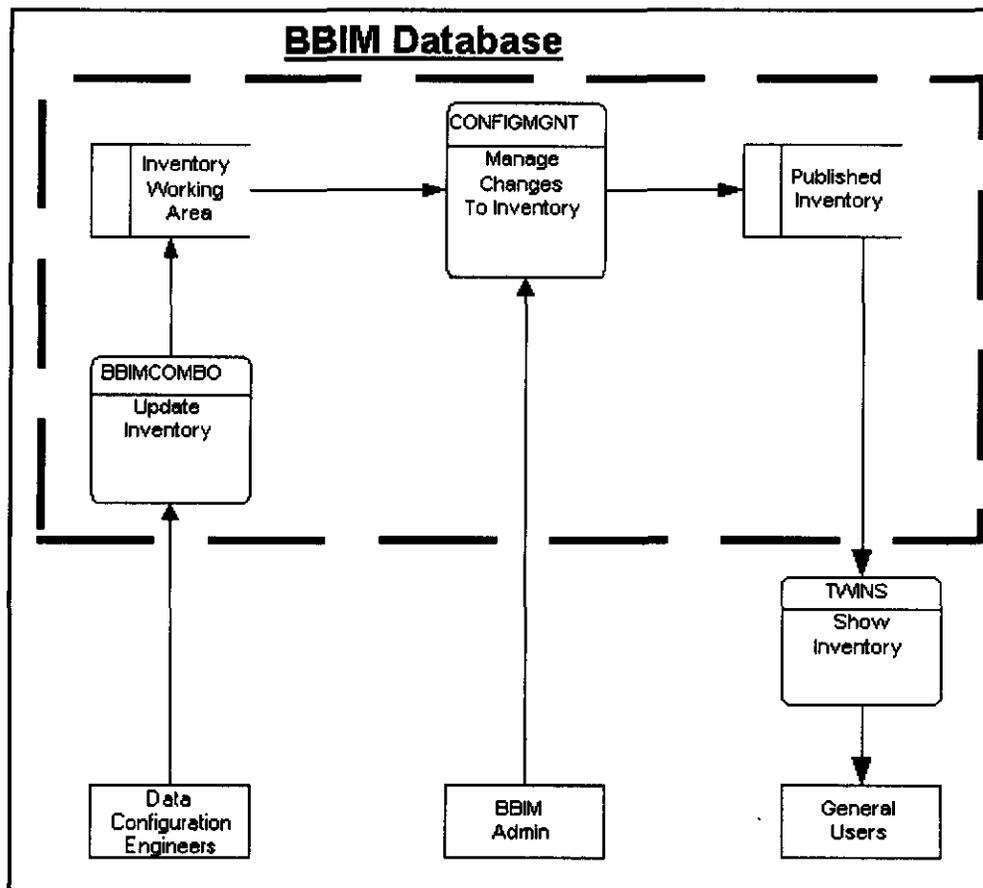
6.0 CONFIGURATION MANAGEMENT (CONFIGMGNT)

The Best-basis Inventory system actually consists of two data areas:

- (1) The **Published Area** contains the official inventory, which is approved and released to the public.
- (2) The **Working Area** is employed when users are adjusting the inventory, but are not ready to officially release the changes.

BBIMCOMBO allows authorized users to change inventory data in the Working Area. Another Access program called CONFIGMGNT manages this process and then releases inventory changes to the Published Area. This chapter discusses CONFIGMGNT. The configuration management modules are illustrated in Figure 6-1.

Figure 6-1. BBIM Configuration Management



Data Configuration Engineers are BBIM data experts, who make decisions concerning the Best-Basis inventory. If they decide to change values in the inventory, they will typically make the changes in the BBIM Working Area, and then, subject to a peer review, the changes will be released to the public in the Published Area. The Data Configuration Engineers make the changes via the Microsoft Access application called BBIMCOMBO.

Once a change is made in the working area, a data configuration engineer will “lock the data” so that no one else can alter the change. This is done by CONFIGMGNT. When this happens, the associated data is *locked*. The change is said to be *pending*. If another data configuration engineer tries to change locked data, BBIMCOMBO will not allow it.

If the change is approved, the BBIM Administrator uses CONFIGMGNT to copy the change into the published area for general viewing, and the associated data in the work area will typically revert back to the normal state of being *unlocked*.

Changes in the work area can cycle through three different states.

1. *Unlocked* –

Authorized Data Configuration Engineers are allowed to change the data.

2. *Pending* –

A change has been entered and is awaiting review. No one can inadvertently alter the associated data without changing the tank status to unlocked.

3. *Published* –

The associated data in the work area are locked.

The change has been approved and moved into the published area.

6.1 WORK UNITS

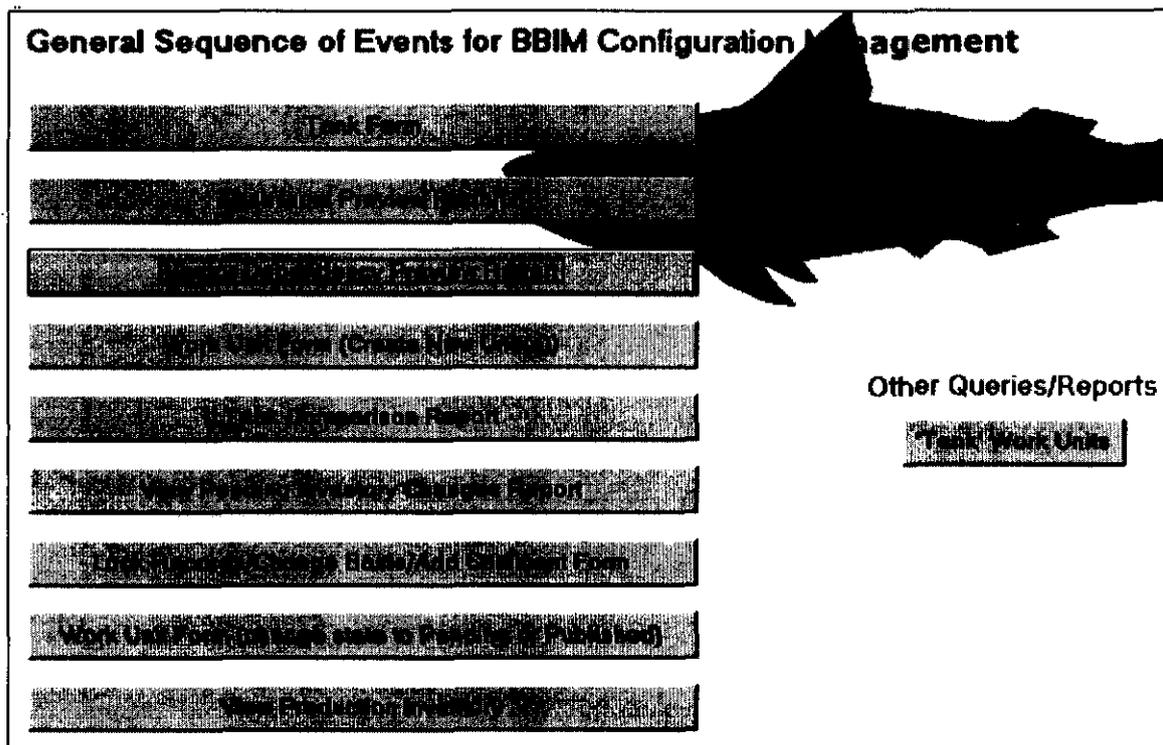
A change to the inventory may involve several elements (tanks and vectors). A group of elements involved in a change is called a *work unit*. For example, if a value in a vector is to be changed, that vector and every tank it affects are part of the same work unit. If data configuration engineers want to protect a change in the work area (for example, to make that change *pending* for approval) they must lock up that work unit. CONFIGMGNT manages this process.

Once a work unit is created and its state is *unlocked* (the initial state of any work unit is *unlocked*), then its members, tank(s) and vectors(s), may be modified. When the modifications are complete, the state of the work unit is changed to *pending*. When a

work unit is in the pending state, no modifications can be made to its members (they are *locked*). At this point, the data are reviewed and can follow these paths:

1. Approved: the work unit is *published* which causes the tank data to be copied over into the published area for general viewing; the work unit is deleted (archived); its members return to a *locked* state.
2. Not approved: work unit can be changed back to "unlocked" where more data modification to its members may be performed.

Figure 6-2. Main Configuration Management Screen



The buttons on the CONFIGMGNT window shown in Figure 6-2 are laid out to follow the process of managing a change to the inventory.

1. Ascertain the status of the inventory by examining the *Tank Form*, the *Tank Input Preview Report*, and the *Vector Dependency Preview Report*.
2. Use BBIMCOMBO to make the desired changes in the work area.
3. For each proposed change identify a work unit with the *Work Unit Form* (see previous discussion). Lock the changed data as *pending*.
4. Designate that you do not want to have inventory changes *forced* into the publishing area, if the new value deviates more than 1% from the previous value.

5. Track the status of pending changes with the *Tank Comparison Report* and/or *View Pending Inventory Changes Report*.
6. Use the *Lock Records/Change Basis/Add Comment Form* module to perform the special procedures required to publish changes.
7. Use the *Work Unit Form* to publish your changes after they have been approved.
8. If the relative percent difference (RPD) between any constituent inventory in the BBIM working area and the inventory value in the BB_Published area is greater than 1%, you may want the CONFIGMGNT tool to use the BBIM working area value anyway. You can do this by setting the publication Update flag to "Force". "Force" is a checkpoint in the publication procedure to confirm or validate the inventory changes. Once you are sure the change is valid, you can publish it.

6.2 PREVIEW REPORTS

This section describes the first three items on the main form of CONFIGMGNT. They provide data that you can use before locking up change data.

Tank Form

The **Tank** form allows the data configuration engineers to view and enter high-level data for a selected tank. Data configuration engineers can view or change data about the associated tank's document, document release date, and/or the effective inventory date for that tank. You can use this form to see when a tank inventory was last updated, or to find the title of a tank inventory document.

Tank Input Preview Report

The **Tank Input Preview** report shows the name and handle of all the vectors that were used to describe the inventory of the selected tank. A *vector handle* is a unique label assigned to each vector by the BBIM tool.

Vector Dependency Preview Report

The **Vector Dependency Preview** report shows the name of all tanks whose inventories are linked to the selected vector. This report is useful for identifying all tanks that depend upon the selected vector. View this report to assess the overall impact before revising any vector information. This report identifies tanks that are locked.

6.3 WORK UNIT FORM (CREATE NEW UNIT(S))

The **Work Unit** form is the first major form in the change control process. Use this form, shown in Figure 6-3, to identify vectors and tanks in the working area that are being changed, and which need to be locked.

Each vector, and its dependent tanks, makes up a work unit. If a tank inventory is the only thing being changed, the tank will be the only item in the work unit. Currently, that is typically the case. As mentioned previously, a work unit is either *Unlocked*, *Pending*, or *Published*, as designated by the *State* of the work unit.

Each work unit is recorded in the *Change Control Board (CCB) Log Book*. On the work unit form, the user records the *CCB Log* number, the *Title* of the change, a *Description* of the change, and a *Justification* for the change. The *Impact* field is free-form text that usually describes the scope of the change – for example, the number of elements affected by the change. At the time of this writing, the *Impact* of every change recorded is “Single Tank”. Comments can be entered into the *Comment* field. Currently, standard practice is to place the tank name in this field.

Figure 6-3. Work Unit Form

State	Pending	WU_ID	28
CCB Log	CCB-070-011	Last_Updated_On	99 11 22 57 AM
Title	Codification Phase II	Last_Updated_By	baune
Description	Reconciliation of BBIM Tool content with the issued Tank		
Justification	Correct mathematical, decay, and protocol errors in the B		
Impact	Single Tank		
Comment	241-AP-102		
Work Unit Members			
Member ID	Member	Member	Member
	241-AP-10		3/25/99 8:53:35 PM
			28 (AutoNumber)

Read-only fields are highlighted in turquoise. These are fields that are filled in by the computer. For example, the computer assigns its own identifying number to each work unit and shows the number in the *WU_ID* field. Similarly, the computer tracks the date the work unit was *Last_Updated_On* and whom it was *Last_Updated_By*.

The **Work Unit Members** subform tracks each item (member) in the work unit. The work unit *Member Type* is either “vector” or “tank”. Currently, all members are tanks. The *Member ID* field records the name of the tank (or the name of the vector).

If a work unit consists of a vector and all of its associated tanks, the vector is called a *Driver* to the tanks, and would be identified in the *Driver* fields. Currently, there are no changes that involve vectors, and the *Driver Type* and *Driver ID* field are always blank.

The computer updates data in the subform for each Work Unit Member.

Added_To_Unit_On records when the member unit was created.

WU_ID is the computer generated ID for the work unit

WUM_ID is the computer generated ID for the work unit member.

If you change a Work Unit state to *pending*, other users cannot change those elements (which still reside in the working area).

6.4 PENDING CHANGES REPORTS

When a change request is first set to a *pending* state, normally the BBIM Tool does not automatically allow data into the public area if the data will cause a change in inventory greater than 1%. This *Update Mode* is called *Default*. The operator must verify that the data is correct and must *force* the data into the published area.

You can view the status of pending changes from the following reports.

Tank Comparison Report

This report compares pending constituent concentrations against the published values for a specific tank and shows the *Update Mode* for each analyte. Data are arranged alphabetically by analyte and reports only standard analytes.

View Pending Inventory Changes Report

This report is similar to the **Tank Comparison** report, except constituents are grouped by *Update Mode: Forced, Default, or Locked*.

6.5 SPECIAL PROCEDURE FOR PENDING DATA

Occasionally, special procedures are needed to publish changes. Most of this is handled through the *Lock Records/Change Basis/Add Comment Form* module. This module brings up a form that asks you to select a tank. Only tanks with pending changes are shown.

After you select a form, CONFIGMGNT will pause while it collects the data and then will bring up a spreadsheet showing all analytic inventories for that tank (and even constituents without pending changes). Some of the data in the spreadsheet cannot be changed, but you can change the following columns of data. Since this is a large spreadsheet, the following sample in Figure 6-4 is presented in two pieces.

Figure 6-4. Pending Inventory Changes Report

Can_Num	BBIM Inv	PUB Inv	RPD	BBIM Comment	PUBLISHED Comment	Update Date	Justification	Tank	BBIM CCB Leg	Unit	PUB Source
Ai	6.46E+04 S/E	6.02E+04 S/E	7.08	Upper bounding estimate			Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM
Bi	1.44E+02 S/E	4.43E+02 M	101.6				Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM
Ce	6.44E+02 S/E	6.43E+02 S/E	2.89				Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM
Cl	1.10E+04 S/E	9.59E+03 S/E	13.49				Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM
TiO ₂	9.13E+04 S/E	9.94E+04 S/E	8.58				Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM
Cr	4.76E+03 S/E	6.00E+03 S/E	23.17	Upper bounding estimate	Sludge only		Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM
F	1.10E+03 S/E	3.46E+01 E	187.7				Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM
Fe	1.43E+03 S/E	1.46E+03 S/E	2.45				Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM
Hg	8.00E+00 E	0.00E+00 E	0		Simran (1998)		Rev. BBIM to reflect new sample date.	241-U-102	CCB-102	kg	BBIM

Can_ID	BBIM Effective Date	PUB Effective Date	BBIM Document	PUB Document	BBIM Release Date	PUB Release Date	Justification	Sort Order
7429-90-5	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	10
7440-69-9	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	20
7440-70-2	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	30
16987-00-6	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	40
189	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	50
7440-47-3	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	60
16984-48-8	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	70
7439-99-6	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	80
7439-97-6	2/1/2000	5/31/1997	AUTO-TOR	HNF-SD-WM-ER-618 Rev. 0B		9/25/1998	Rev. BBIM to reflect new sample date, transactions, and	90

BBI Basis

You can override the *basis* that is computed by the BBIM Tool, by changing the designation in this column. The new basis is stored in the work area and will not show up until after the data have been published.

BBIM Comment

This field allows you to enter comments in the working area. The comment will be copied over to the published area when the change is published (if the *Update Mode* is *Force*).

Update Mode

Normally, the BBIM Tool will not allow an analytic inventory into the published area if the RPD is greater than 1%. After verifying the new result, the operator overrides this feature by setting the designation in this field to *Forced*. If you do not want to override the previously published data for this analyte, under any circumstances, you can set this field to *Locked*. Each analyte for each tank has its own update mode setting.

Justification

If you change the *Update Mode* to anything but *Default*, you must explain this action in the *justification* field provided on the form. Default does not need to be resolved.

Hydroxide

If you close the spreadsheet, another form will display. This form allows you to change the *Update Mode* for hydroxide. Once again, you are required to provide justification if you change the *Update Mode* to anything other than default.

Note: Filling in the *justification* field is an administrative requirement.

6.6 PUBLISHING CHANGES

Work Units are published by accessing the **Work Unit** form (by either button on the main menu) and by then setting the work unit's state to *Published*.

The entire procedure is:

1. Go from *Unlocked* to *Pending*
2. Exit the form
3. Reenter the form
4. Go from *Pending* to *Published*.

6.7 VIEW PRODUCTION INVENTORY

To view the published inventory, press the *View Production Inventory* button on the Main Form. A spreadsheet report will appear, showing the total of each analyte for each tank.

Besides the inventory itself, this report shows the basis of the inventory and the last change that affected the constituent. The log number, work unit id, update mode, comment, justification, change date, and effective inventory date are all shown, for the most recent change.

6.8 TANK WORK UNITS

To see a list of all work units in progress, press the *'Tank' Work Units* button on the Main Form. A spreadsheet report will appear, showing each work unit in progress – both pending and unlocked. This report shows the work unit id, the state, the log number, title, description, justification, comment, last update, and the affected tank or vector, for each work unit.

7.0 TECHNICAL DESCRIPTION

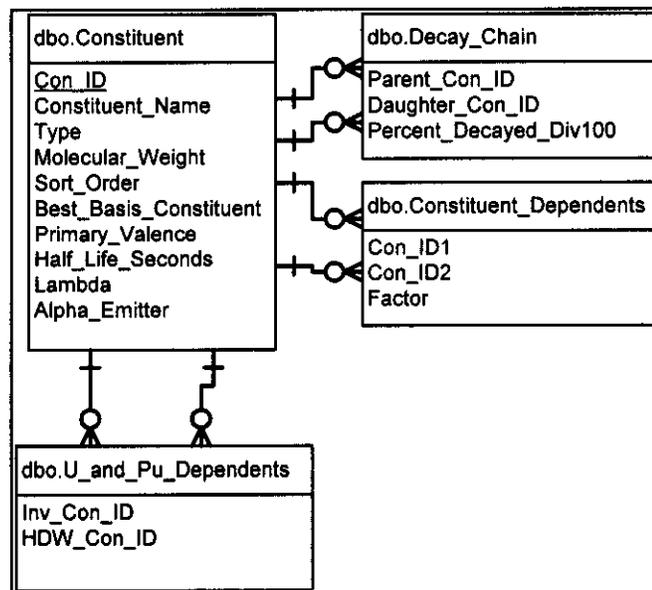
This section describes the formulas and data structures used by the BBIM Tool in order to better understand exactly how calculations are performed, and what they mean.

First, the major database constructs, or tables are described. “Entity-Relationship,” or “data model” diagrams are shown to depict the relationships between the tables. Next, the database calculations are described – first at the component level, and then at the total tank level. This is done because, while most calculations are done at the component level and then simply added together to come up with the total tank inventory, there are calculations that are only done at the total tank level.

7.1 CONSTITUENTS

The words constituent and analyte are often used interchangeably at Hanford. The BBIM database mostly uses the term **constituent**. Figure 7-1 illustrates the relationship of several BBIM database tables that describe constituents. All four of these tables store relatively constant information that is used in later calculations.

Figure 7-1. Data Structure for Constituents



The main table describing constituents is called **Constituent** (see Table 7-1). It is an important table. The contents of some of the columns are shown below.

Table 7-1. Assorted Fields from Constituent Table (3 sheets)

Constituent_Nam	Type	Be2_Emit_Constituent	Primary_Valence	Alpha_Emit
3H	Radionuclide	Y		
137Cs	Radionuclide	Y		
90Y	Radionuclide	Y		
90Sr	Radionuclide	Y		
60Co	Radionuclide	Y		
P	Chemical	Y		
SiO3	Chemical		-2	
Te	Chemical			
234U	Radionuclide	Y		-1
106Ru	Radionuclide	Y		
134Cs	Radionuclide	Y		
233U	Radionuclide	Y		-1
244Cm	Radionuclide	Y		-1
238Pu	Radionuclide	Y		-1
63Ni	Radionuclide	Y		
242Pu	Radionuclide	Y		-1
226Ra	Radionuclide	Y		
237Np	Radionuclide	Y		
241Pu	Radionuclide	Y		
240Pu	Radionuclide	Y		-1
99Tc	Radionuclide	Y		
232U	Radionuclide	Y		-1
125Sb	Radionuclide	Y		
PO4	Chemical	Y	-3	
231Pa	Radionuclide	Y		
59Ni	Radionuclide	Y		
155Eu	Radionuclide	Y		
241Am	Radionuclide	Y		-1
152Eu	Radionuclide	Y		
14C	Radionuclide	Y		
NO3	Chemical	Y	-1	
NO2	Chemical	Y	-1	
NH4	Chemical			
SO4	Chemical	Y	-2	
227Ac	Radionuclide	Y		
243Am	Radionuclide	Y		-1
129I	Radionuclide	Y		
239Pu	Radionuclide	Y		-1
235U	Radionuclide	Y		-1
228Ra	Radionuclide	Y		

Table 7-1. Assorted Fields from Constituent Table (3 sheets)

Constituent Nam	Type	Is a HLE constituent	Primary Valence	Alpha Emitter
242Cm	Radionuclide	Y		-1
154Eu	Radionuclide	Y		
229Th	Radionuclide	Y		
151Sm	Radionuclide	Y		
93Zr	Radionuclide	Y		
243Cm	Radionuclide	Y		-1
79Se	Radionuclide	Y		
126Sn	Radionuclide	Y		
Cl	Chemical	Y	-1	
F	Chemical	Y	-1	
TIC as CO3	Chemical	Y	-2	
CO3	Chemical	Y		
S as SO4	Chemical	Y		
Pd	Chemical			
Si as SiO3	Chemical			
Oxalate	Chemical			
236U	Radionuclide	Y		-1
CN	Chemical			
EDTA	Chemical			
Al	Chemical	Y	3	
Fe	Chemical	Y	3	
La	Chemical	Y	3	
Pb	Chemical	Y	2	
Li	Chemical			
Mg	Chemical			
Mn	Chemical	Y	4	
Hg	Chemical	Y	2	
Mo	Chemical			
Nd	Chemical			
Ni	Chemical	Y	2	
Pu	Chemical			
K	Chemical	Y	1	
Rb	Chemical			
Rh	Chemical			
Pr	Chemical			
Ru	Chemical			
Si	Chemical	Y	-2	
Ag	Chemical			
Na	Chemical	Y	1	
Sr	Chemical	Y	2	
Ta	Chemical			
Tl	Chemical			
Th	Chemical			
Ti	Chemical			
W	Chemical			

Table 7-1. Assorted Fields from Constituent Table (3 sheets)

Constituent_Nam	Type	Rad Emitter	Primary Valence	Alpha Emitter
Sb	Chemical			
As	Chemical			
Ba	Chemical			
Be	Chemical			
B	Chemical			
Cd	Chemical			
Ce	Chemical			
Cs	Chemical			
Cr	Chemical	Y		3
Co	Chemical			
Cu	Chemical			
UTOTAL	Chemical	Y		6
V	Chemical			
Y	Chemical			
Zn	Chemical			
Zr	Chemical	Y		4
Bi	Chemical	Y		3
Ca	Chemical	Y		2
NH3	Chemical			
S	Chemical			
P as PO4	Chemical	Y		
Water	Water			
Se	Chemical			
137mBa	Radionuclide	Y		
113mCd	Radionuclide	Y		
243/244Cm	Radionuclide	N		
FeCN	Chemical			
OH	Chemical	Y		-1
93mNb	Radionuclide	Y		
239/240Pu	Radionuclide			
232Th	Radionuclide	Y		
TIC	Chemical	Y		
TOC	Chemical	Y		-0.33
TotalAlpha	Radionuclide			
238U	Radionuclide	Y		-1

7.1.1 Type

Constituents are classified by BBIM as either *Chemical* or *Radionuclide*.

7.1.2 Best_Basis_Constituent_Flag

If a constituent is considered an approved best-basis constituent that is to be reported by the BBIM database, the **Best_Basis_Constituent_Flag** is set to *Y* (meaning yes, it is to be reported). This flag is used primarily by queries and reports so only the standard best-basis constituents are visible. A new best-basis constituent can be established by setting this flag and assigning the other fields (Molecular Weight, Primary Valence, Alpha Emitter, etc).

7.1.3 Primary_Valence

Primary_Valence is used for computing the amount of hydroxide in the tank, as discussed previously. If a constituent has a non-null **Primary_Valence**, it is considered an anion or a cation and is used in the charge balance calculations. If the **Primary_Valence** is null, the constituent is not considered in the charge balance calculations.

7.1.4 Alpha_Emitter

This field is used by the Total Alpha HDW Isotopic Distribution software to identify which constituents are alpha-emitting radionuclides. If a constituent is an alpha emitter, the **Alpha_Emitter** column is set to -1.

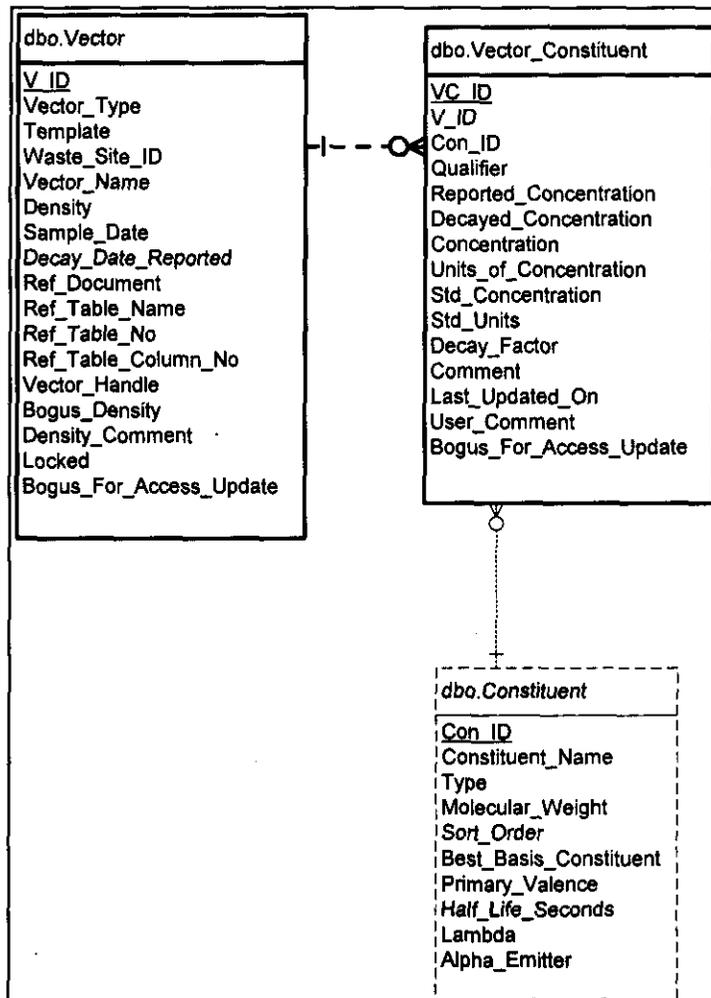
7.1.5 Molecular_Weight, Half_Life_In_Seconds, Lambda, and Sort_Order

In addition to the values shown above, the **Constituent** table stores values for **molecular weight**, **half-life in seconds**, and **Lambda** (half-life) for each constituent. The **Sort_order** and **Con_id** values are used internally by the computer and are not of concern to the user.

7.2 VECTORS

When the term “vector” is used, it is generally taken to include all of the constituents, their concentrations, engineering units, and associated metadata. In point of fact, in the database there are two tables that contain the information normally associated with the term “vector”: the **Vector** table and the **Vector_Constituent** table (see Figure 7-2). When vectors are created, the BBIM database saves each constituent concentration in a separate record in the **Vector_Constituent** table. The **Vector** table, on the other hand, contains all of the metadata regarding the Vector. These metadata are described following.

Figure 7-2. Vector and Vector_Constituent Structures



7.2.1 Vector_Type

Vector_Type is a required field. It designates whether the data came from, as shown in Table 7-3. The allowable vector types are shown in the following table.

Table 7-2. Vector Type

Vector_Type	Data was obtained from:
Sample	Laboratory sample analysis
HDW	A model
Process Knowledge	The concentrations are based historical knowledge of the processes that produced the waste

A vector cannot contain mixed data, such as a combination of data from sample analysis and from process knowledge.

7.2.2 Template

A **Template** is a waste type that will be used repeatedly. If a vector is used to construct a template, the template name must be entered in this field. In order to be selected from the pull-down list, the template name should be identified before hand. If the vector will not be used as part of a template, select *N/A*.

7.2.3 Vector_Name

Vector Name is a required field. A vector must be assigned a name (typically it would be the column name if extracted from a table in a document).

7.2.4 Vector_Handle

Vector_Handle is a unique identifier for a vector; it is computed automatically for you by BBIMCOMBO. It has the form: TFFNNN##, where T is the **Vector_Type** (S/H/P), FF is the tank farm (e.g., A, AX), NNN is the tank number (e.g., 101) or Vector **Waste_Site_ID** from which the sampled or modeled material came from or represents, and ## is an integer incrementally assigned to new vectors for a vector **Waste_Site_ID**.

7.2.5 Density

Density is a required field – so that mass concentration can be adjusted to volumetric concentration when required. Standard density units of grams/milliliter are implied. If the density is unknown, enter an estimated amount and set **Bogus_Density** equal to yes. This will flag the density as an estimate so a more precise value can be entered later on.

In the meantime, the density will allow BBIM to use the vector. (The BBIM database insists that density be entered). **Density** is stored (in g/ml) in the **Vector** table. The density is applied to all concentrations in the vector to compute inventory.

7.2.6 Bogus_Density

This is a flag set by the user, indicating whether **Density** is a quality number. If not, **Bogus_Density** will be set to *True*.

Notice that some of the more complicated calculations are performed later when a tank waste component is created or updated.

7.2.7 Density_Comment

This optional field is used to document where the density is referenced. Often, the Density is reported in the same document table from which the rest of the vector data came from and so is left blank.

7.2.8 Sample_Date

The date when sampling was done (for sampled data only).

7.2.9 Decay_Date_Reported

The date that the reported concentrations have been decayed from (the decay logic uses this date to start the decay, and decays to the **Standard_Decay_Date**). Thus, the BBIM does not assume all reported concentrations are not adjusted to some decay date.

7.2.10 Ref_Document

The name of the document (SD name for example) from which this vector data were extracted.

7.2.11 Ref_Table_Name

Name of the table from which numbers were taken.

7.2.12 Ref_Table_No

Number of the table from which numbers were taken (e.g., 2-2).

7.2.13 Ref_Column_No

Column number containing the numbers from the table.

7.3 VECTOR_CONSTITUENT

Once the vector and its source document are described, you can identify the constituents and identify the concentrations in the **Vector Constituents** sub-form. The computer updates the *vc_id* column on the sub-form automatically.

The following paragraphs describe the main fields in the Vector_Constituent table:

7.3.1 Qualifier

This value qualifies the concentration of the constituent. Some qualifiers are used by the database to choose between different vector concentrations for the same waste component. Acceptable values are:

- < concentration is less than the detection limit
- <DL concentration is less than the detection limit
- NR concentration is not reported
- NA value is not applicable
- Null the qualifier may not be entered

7.3.2 Reported_Concentration

This is the concentration reported in the source document and entered by the user.

7.3.3 Units_Of_Concentration

These are the concentration units reported in the source document and entered by the user. BBIM converts many different types of units as described below.

7.3.4 Std_Units

The **Std_Units** are a subset of the allowed **Units_Of_Concentration** values, which BBIM uses so that calculations are consistent. At the time of this writing, standard units are:

- ug/g*
- uCi/g*

7.3.5 Std_Concentration

The BBIM tool converts each **Reported_Concentration** to standard units and stores the result in **Std_Concentration**.

7.3.6 Decayed_Concentration

This is the estimated concentration of the constituent on the **Standard_Decay_Date** (currently January 1, 1994). The **Std_Concentration** of each constituent of type *Radionuclide* is adjusted to what it would have been on the **Standard_Decay_Date** and the resulting value is stored in this field. The calculations are discussed below.

$$\text{Decayed_Concentration} = \text{Std_Concentration} * \text{Decay_Factor}$$

7.3.7 Decay_Factor

To compute the **Decay_Factor** we must know the intended date of the measurements (or estimates). This is called the **Decay_Date_Reported**. It is the same for all concentrations that are reported within the same vector and is stored in the **Vector** table. Using this date, we compute the difference, in days, between it and the **Standard_Decay_Date**.

$$\text{Ndays} = \text{Standard_Decay_Date} - \text{Decay_Date_Reported}$$

Notice that **Ndays** will be negative if the reported date is greater than the standard decay date. This is as it should be, so that the formula below can work properly.

To simplify the decay calculations, we can take the half-life of each radionuclide (usually expressed in seconds) and convert it into a number called **Lambda** (which is typically expressed in 1/days). In the calculation below $\ln(2)$ is the natural log of 2.

$$\text{Lambda} = \text{Ln}(2) / (\text{half-life_in_seconds} / 86400)$$

For most radionuclides, we only compute the decay factor for first-order decay – compensating for the amount of radionuclide that is lost due to decay.

$$\text{Decay_Factor} = e^{**} (-\text{Lambda} * \text{Ndays})$$

(** is the symbol used for exponentiation)

Second order decay factors are computed for daughter constituents that are listed in the **Constituent_Dependents** table. Currently, there are only 4 daughter constituents – Ra-228, Am-241, Ac-227, and Nb-93m.

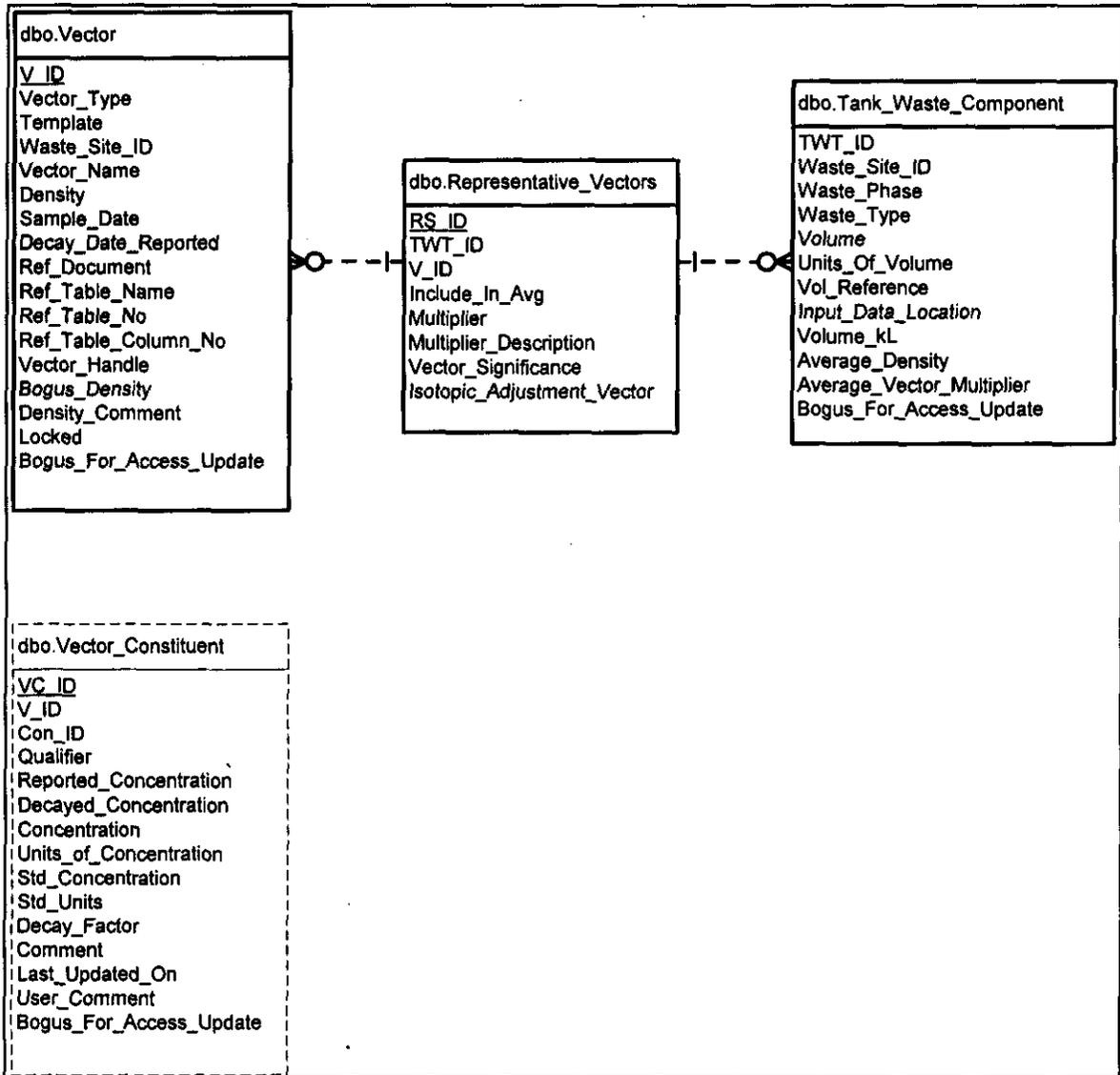
For each daughter in **Decay_Chain**

$$\text{Second_Order_Decay_Factor} = (\text{Decay_Factor_of_daughter} + ((\text{Daughter.Lambda}) / (\text{daughter.lambda} - \text{parent.lambda})) * (\text{Parent_Decay_Factor} - \text{Daughter_Decay_Factor}))$$

7.4 REPRESENTATIVE VECTORS

The **Representative_Vectors** table provides a many-to-many link between the **Vector** table and the **Tank_Waste_Component** table. A vector can be associated with many tank waste components and a tank waste component can be associated with many vectors.

Figure 7-3. Representative Vectors



7.4.1 Include_In_Avg

This value is *Y* (yes) if this vector is to be averaged together with other vectors to make an average vector for this waste tank component. Notice that average vectors are not stored in the vector table – only the vectors that combine to make up the average are stored. Instead, the final averaged values are stored in the **Tank_Waste_Inventory** table as explained later on.

7.4.2 Multiplier

Each concentration in the vector is multiplied by the **Multiplier** before the resulting inventory number is stored in the **Tank_Waste_Inventory** table. Normally, the **Multiplier** will be equal to one. However, sometimes an entire vector of constituents may become more or less concentrated (because of evaporation or dilution during a waste transfer, as an example).

7.4.3 Vector_Significance and Isotopic_Adjustment_Factor

These fields are artifacts of previous programs, and should be ignored.

7.5 TANK_WASTE_COMPONENT

The **Tank_Waste_Component** table stores the id and volume of each waste component.

7.5.1 Waste_Type

The **Waste_Type** field can be used to assign a name to any tank waste component that is characterized from process knowledge, rather than measurements. Several tank waste components across the site may be of the same **Waste_Type**.

7.5.2 Volume

The numeric value of the volume for the tank waste component.

7.5.3 Units_Of_Volume

Usually *kL* but could be *kgal*.

7.5.4 Vol_Reference

This field is used when the volume was obtained from a document other than the best-basis document for the tank. In such a case, this field will store the name or document number from which the volume was obtained.

7.5.5 Input_Data_Location

During the loading of data into the BBIM database, tables are extracted from the electronic versions of best-basis documents and saved for future use.

Input_Data_Location is the path and filename where these tables are stored relative to the `\\TCD_DOCS\best_basis_baseline` file share.

7.5.6 Average_Density

When **Density** is averaged across each vector that was used to create an average vector, the value is stored here. When an average vector was not computed, this field is meaningless.

7.5.7 Average_Multiplier

The multiplier is averaged across each vector that was used to create an average vector, and the value is stored here. When an average vector was not computed, this field is meaningless.

7.5.8 Average Vector Calculations

The following formula demonstrates how **Average_Vector_Density** and **Average_Vector_Multiplier** are calculated.

IF **Average_Vector_Is_Created** THEN

Average_Vector_Density = average of the component vector densities

Average_Vector_Multiplier = average of the component vector multipliers

7.6 SIMPLE RATIO CALCULATIONS: CONSTITUENT DEPENDENTS

As mentioned previously, BBIM often takes advantages of certain key ratios, which allow us to predict the amount of one isotope by measuring the concentration of another. These constant relationships are stored in the **Constituent_Dependents** table.

At the time of this writing there were five dependencies stored:

Table 7-3. Constituent Dependents

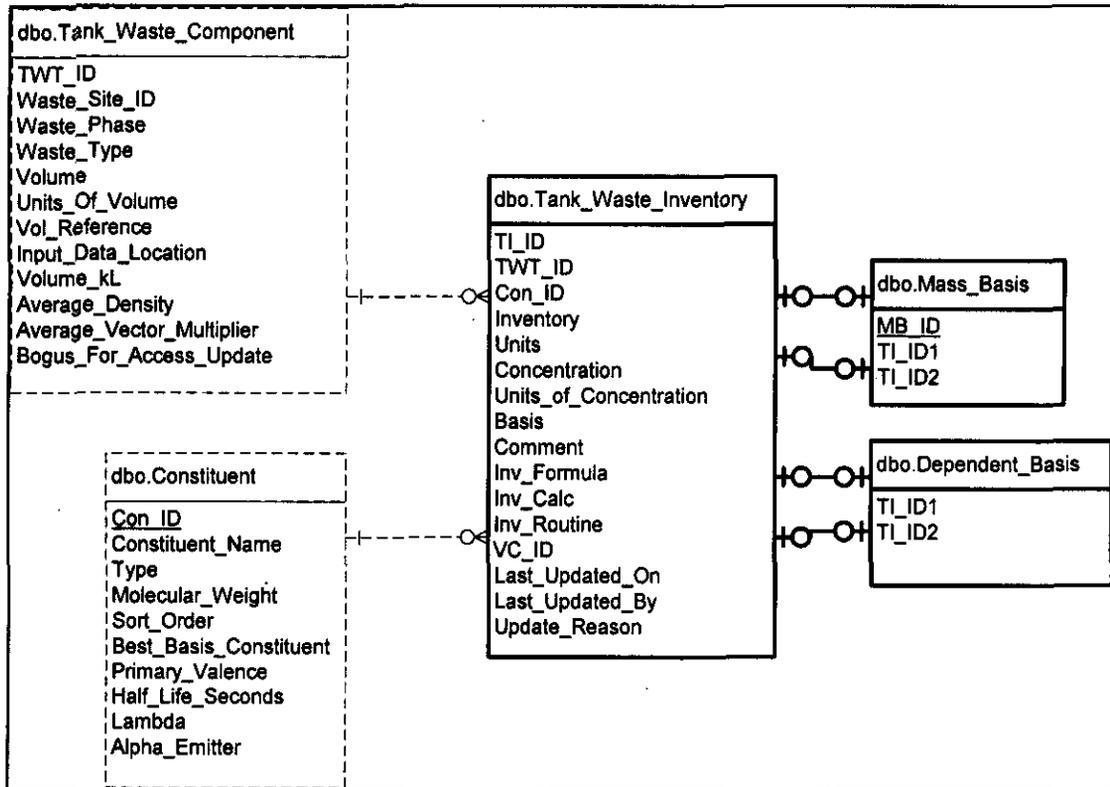
Constituent 1	Constituent 2	Factor (const1 /const2)
Y-90	Sr-90	1.0
Ba-137m	Cs-137	0.946
Cm-243	CM-243/244	0.04
Cm-244	CM-243/244	0.96
Sr	Sr-90	2.4436E-05

The last dependency, Sr and Sr-90, is a special case in which curies are converted to kilograms. Calculations are explained in detail in a later section that discusses Vectors.

7.7 COMPONENT INVENTORY CALCULATION AND BASIS SETTING

Each record in the **Tank_Waste_Inventory** table describes the inventory for a given constituent in a given waste *component* – not in the whole tank, but just in the component. The sum of all components would equal the total tank inventory.

Figure 7-4. Tank Component Inventory



Tank_Waste_Inventory records are created by using the **Radio Button** form. Often, a user will gather several vectors and will then select a value from whichever vector is preferred, on a constituent-by-constituent basis.

7.7.1 Phases

Each row in the **Tank_Waste_Component** table corresponds to a block of waste in a tank. Each block of waste belongs to a class of waste, called a **Waste_Phase**. At the time of this writing, the allowed waste phases are:

Supernatant
Salt Cake
Sludge

7.7.2 Concentration

This field stores the concentration selected (e.g., on the **Radio Button** form) for the constituent. If the constituent is of type *radionuclide*, the concentration is pulled from **Vector_Constituent:Decayed_Concentration**, otherwise it is pulled from **Vector_Constituent:Std_Concentration**.

```
If ConstituentType == Radionuclide Then
    Tank_Waste_Inventory:Concentration
    = Vector_Constituent:Decayed_Concentration
Else Tank_Waste_Inventory:Concentration
    = Vector_Constituent:Std_Concentration
```

Units of concentration are copied over in a similar fashion.

7.7.3 Inventory

Standard **Inventory** units are *kg* or *Ci*. The BBIM accepts concentrations in several different forms and converts them to mass or curies as follows:

For solid units of concentration (e.g., micro-grams/gram or Curies/gram)
Inventory = Concentration * Vector:Density * Tank_waste_component:Volume

For liquid units of concentration (e.g., micro-grams/liter or Curies/liter)
Inventory = Concentration * Tank_waste_component:Volume

For molar units of concentration (e.g., micro-grams/mole or Curies/mole)
Inventory = concentration * molecular-weight * volume

7.7.4 Component Basis Setting

Each inventory record is assigned a **Basis** from the vector that provided the concentration for that constituent. If an average vector was used, the **Basis** is set equal to **Sample Average**.

Inv_Formula, and **Inv_Calc**, store the text version of the formulas and calculations that are displayed in the detailed calculation report.

The formulas above apply to most constituents, but there are many special cases, as explained below. The computer code that implements these special cases is triggered whenever associated records are inserted, updated, or changed.

7.7.5 Simple Ratios: Constituent Dependents

If Sampling and Process Knowledge inventory numbers are unavailable for a constituent, sometimes the concentration can be **calculated** based upon a ratio found in the **Constituent_Dependents** table. The following algorithm is used.

```

FOR a Dependent_Constituent (one that is found in the Dependent_Constituent Table)
  IF (a non-calculated inventory number does not exist for constituent1 ) THEN
    IF (an inventory number does exist for constituent 2) THEN
      Constituent1_Inventory = Constituent2_Inventory * Factor_in_Dependents_Table

```

Whenever the concentration for a constituent is calculated in this way, a record is placed in the **Dependent_Basis** table that points to the original estimate for the constituent (which came from a model) and to the new computed value.

Whenever Sr is computed in this manner from Sr-90, the BBIM database must convert the inventory of Sr-90, which has units of curies, into an inventory number for Sr, which has units of grams. The formula for this conversion is as follows:

```

IF (we have sample based 90Sr, but don't have Sr for a component)
  Sr(kg) = 90Sr(Ci) * .024436 / (Rho (vector) * Vol_kl (component))

```

```

0.024436 = 1/(0.3*136.4*1000)

```

7.7.6 Radioactive Decay

Radionuclides decay over time into other constituents. Thus, the inventory of radionuclides in 1980 will be different from the inventory in year 2000 because of radioactive decay (and other factors). The best-basis inventory is estimated from sampling information that was gathered at many different times. A strategy is used to adjust the radionuclide sampling measurements to a common date, so that results will be consistent.

The **Constituent** table stores a **Half_Life_Seconds** value and **Lambda** for each radionuclide. This allows the database to adjust for decay, as will be described later. **Lambda** can actually be calculated from **Half_Life_Seconds**.

$$\text{Lambda} = \log(2)/(\text{Half_Life_Seconds}/86400)$$

7.7.6.1 Decay Dependents

Radionuclides slowly decay over time into other constituents. Sometimes, this is not important for calculating the inventory (because of the small amounts involved), but sometimes, it is. The **Decay_Chain** table stores decay relationships that are of interest to the BBIM Tool. At the time of this writing, there are only four relationships stored:

Table 7-4. Parent-Daughter Decay Chain Dependents

Parent	Daughter	Percent Decayed Div100
Th-232	Ra-228	1.0
Pu-241	Am-241	0.99998
Pa-231	Ac-227	1.0
Zr-93	Nb-93m	1.0

These relationships are used when computing the inventory, and the calculations involved are discussed later.

First order decay computes the percentage of an isotope that is lost over a certain amount of time, as radioactive decay causes some of the isotope to change into another substance. Second-order decay computes both how much of an isotope is lost, and also how much is gained because of decay from a parent isotope. For example, to compute the second-order decay for Ra-228, we calculate how much Ra-228 is lost to decay, and also how much is gained back again because of decaying Th-232.

7.7.7 HDW Isotopic Distributions: U and Pu Dependents

The **U_and_Pu_Dependents** table is used to perform the HDW isotopic distribution calculations. The column, **Inventory_Constituent** contains a uranium or plutonium isotope constituent name, and the column, **Model_Constituent** contains a constituent name that, in the HDW Isotopic Distribution scheme, is dependent upon the **Inventory_Constituent**.

Table 7-5. Uranium and Plutonium Dependents Table

Inventory Constituent	Model Constituent
Utotal	UTotal
Utotal	U-232
Utotal	U-233
Utotal	U-234
Utotal	U-235
Utotal	U-236
Utotal	U-238
Pu-239/240	Pu-239
Pu-239/240	Pu-240
Pu-239	Pu-238
Pu-239	Pu-240
Pu-239	Pu-241
Pu-239	Pu-242
Am-241	Am-243
Am-241	Cm-242
Am-241	Cm-243
Am-241	Cm-244

In the algorithm displayed below, the following variables are used:

Inv_Con

This constituent is listed in the first column of the **U_and_Pu_Dependents** table. The idea being that if we can find an inventory number for this constituent in the **Tank_Waste_Inventory** table, we can better estimate the value of other isotopes using the HDW model to form a ratio. To apply this technique, the amount of inventory for **Inv_Con** must be stored in the **Tank_Waste_Inventory** table, and it must come from Sampling information or from Process Knowledge.

It is assumed that BBIM will not contain sampled and/or process knowledge values for both *Pu239* and *Pu239/Pu240* in the same vector. If this happens, the *Pu-239/Pu-240* value will take precedence.

HDW_Con:

This constituent is listed in the second column of the **U_and_Pu_Dependents** table. The idea being that we can use **Inv_Con** to compute a value for this constituent. This technique applies only if the **Tank_Waste_Inventory** table does not have a non-calculated inventory value stored for this constituent.

FOR EACH RECORD IN U_and_Pu_Dependents Table

FOR EACH useable Inv_Con entry (see above)

FOR EACH useable HDW_Con entry (see above)

HDW_Con.value = Inv_Con.value * HDW_Con.Model / Inv_Con.Model

Value is the final estimated inventory value.

Model is the inventory estimated in the HDW Model.

7.8 TOTAL TANK INVENTORY CALCULATION

The **Tank_Inventory** table holds a separate record for each constituent in a given tank. Each record holds the tank's inventory for that constituent. Note that the **Tank_Inventory** table and **Tank_Waste_Inventory** table are similar. The first table is for tanks, and the second one is for tank components (which make up the waste contents of a tank).

7.8.1 Total Tank Inventory and Basis Calculations

In fact, the **Tank_Inventory** table is created from the **Tank_Waste_Inventory** table by *summing the component inventories for each constituent*

The total tank Basis for a constituent is normally created from the multiple component bases by concatenating them together. Thus, if a tank has one component with an "S" basis and another with an "M" basis, the total tank Basis would be "S/M" for that single constituent.

Additionally, the following logic applies if some components are created from sample average vectors: if all the vectors that make up the sample average component inventory come from the same tank as the component and their type is 'Sample', then set the **Tank_Inventory** basis to 'S', otherwise set to 'E' (since the average is based upon another tank's sample or the vector is based on something other than a 'Sample' ['Process Knowledge' or other]).

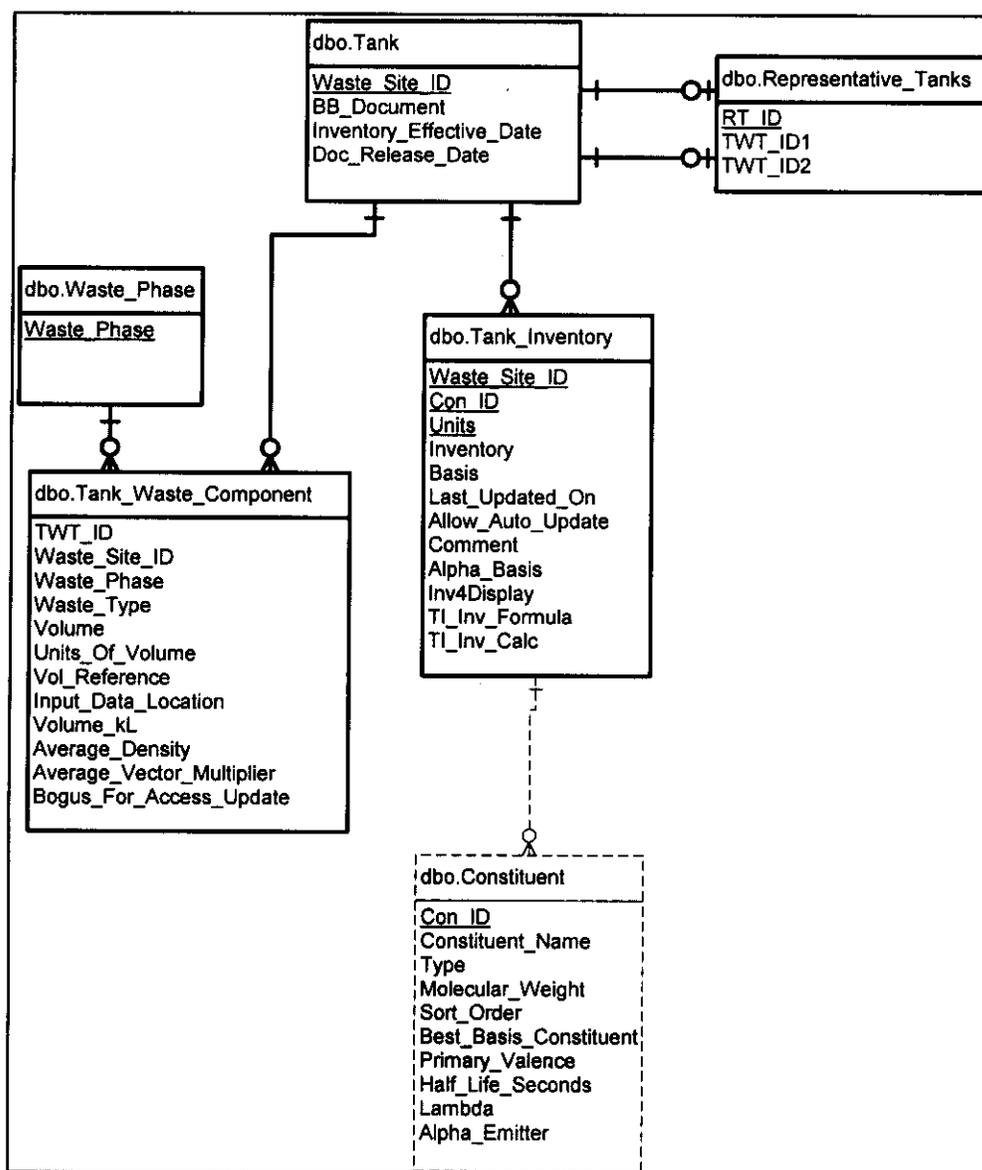
Note in Figure 7-5 that **Tank_Waste_Inventory** is not related to **Tank_Inventory** by a database relationship; however, it is crucial that **Tank_Inventory** be updated faithfully whenever **Tank_Waste_Inventory** changes. In the SQLServer database, this is accomplished by the use of "triggers". A database trigger is analogous to an interrupt

processing routine – it is automatically executed whenever some event occurs. In the case of the database, these events are: Insert/Delete/Update of database records in the **Tank_Waste_Inventory** table. In the BBIM database, there are triggers to handle these events.

7.8.2 Special Handling of '<' Qualifiers

One exception to the normal Basis setting rule applies to the total tank inventories that are based on concentration values having a "<" qualifier. The rule is that if more than 10% of the total tank inventory is based on vector concentrations having a "<" qualifier, then an "S/E" Basis is used instead of the normal Basis and the Tank_Inventory Comment field is set to "Upper Bounding Estimate".

Figure 7-5. Tank Inventory



7.8.3 Total Waste Phase

This is a special phase that is used to over-ride all of the other phases and consequently all other waste components. The logic for this goes as follows:

```

FOR EACH tank,
  FOR EACH constituent_in_the_tank
    IF constituent = hydroxide THEN
      Tank_Inventory_of_hydroxide =
        Sum_of_hydroxide_inventory_across_all_components_in_the_tank
    ELSE (constituent is not hydroxide) THEN
      IF constituent_is_a_component_of_the_“Total_Phase” THEN
        Tank_inventory_of_that_constituent =
          The_inventory_of_that_constituent_in_the_”Total_Phase”
      ELSE (constituent isn’t listed as part of the “Total_Phase”) THEN
        Tank_inventory_of_that_constituent =
          Sum_of_inventories_across_all_components_for_that_tank /
            constituent.

```

7.8.4 Total Alpha

If data exist for the *TotalAlpha* constituent, it may be used as a last resort, when all else fails. This is done by first subtracting all alpha-emitting sample-based values from the gross *TotalAlpha* for the whole tank. Then, the remaining alpha is assigned to any of the previously identified isotopes.

If we have a TotalAlpha measurement for the tank then

```

Known_List           = List of all alpha emitters whose
                        concentrations are known from sampling, `
                        sample-averaging, or process knowledge
Unknown_List        = List of alpha emitters whose concentrations
                        are NOT known from sampling, sample-
                        averaging, or process knowledge
Known_List_Sample   = sum(sample-based alpha from Known_List)
Unknown_List_HDW    = sum(HDW-based alpha from Unknown_List)

NetTotalAlpha       = TotalAlpha – Known_List_Sample
HDWNetTotalAlpha    = Unknown_List_HDW

```

FOR EACH constituent in Unknown_List plus ²⁴¹Pu

```

Inventory = HDW_Isotope * NetTotalAlpha/HDWNetTotalAlpha

```

Note: this algorithm estimates ^{241}Pu even though it is not an alpha-emitter (and is not included in the calculations of **NetTotalAlpha** and **HDWNetTotalAlpha** described above).

Total Alpha calculations are performed over the entire tank as a whole, not by tank component (as most others are calculated).

Note: The alpha-emitting radionuclides used in this procedure are: ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{242}Pu , ^{241}Am , ^{243}Am , ^{242}Cm , ^{243}Cm , and ^{244}Cm .

7.8.5 Hydroxide

Hydroxide is the last constituent calculated, because its inventory is derived from the *Primary Valence Count* of the other constituents (see previous chapters).

Radionuclides are not assigned a valence count. That is to say, their valence count is null. However, *UTOTAL* is listed as a *CHEMICAL* constituent, and it is used during hydroxide calculations and is assigned a *Primary Valence Count* of 6.

Hydroxide must be recalculated whenever inventory data are changed in the BBIM database. However, when data are published, the working area may not always match the published data, so hydroxide must be recalculated for the published area as well.

Hydroxide is the only constituent that is totaled both for the *TOTAL* Waste Component, and all the other components as well.

The procedure for estimating hydroxide is as follows:

Net_Charge = 0

FOR EACH waste component in the tank

FOR EACH constituent in the waste component

**Net_Charge = Net_Charge + inventory (in kg) * 1000 *
primary_valence_count / Molecular_Weight**

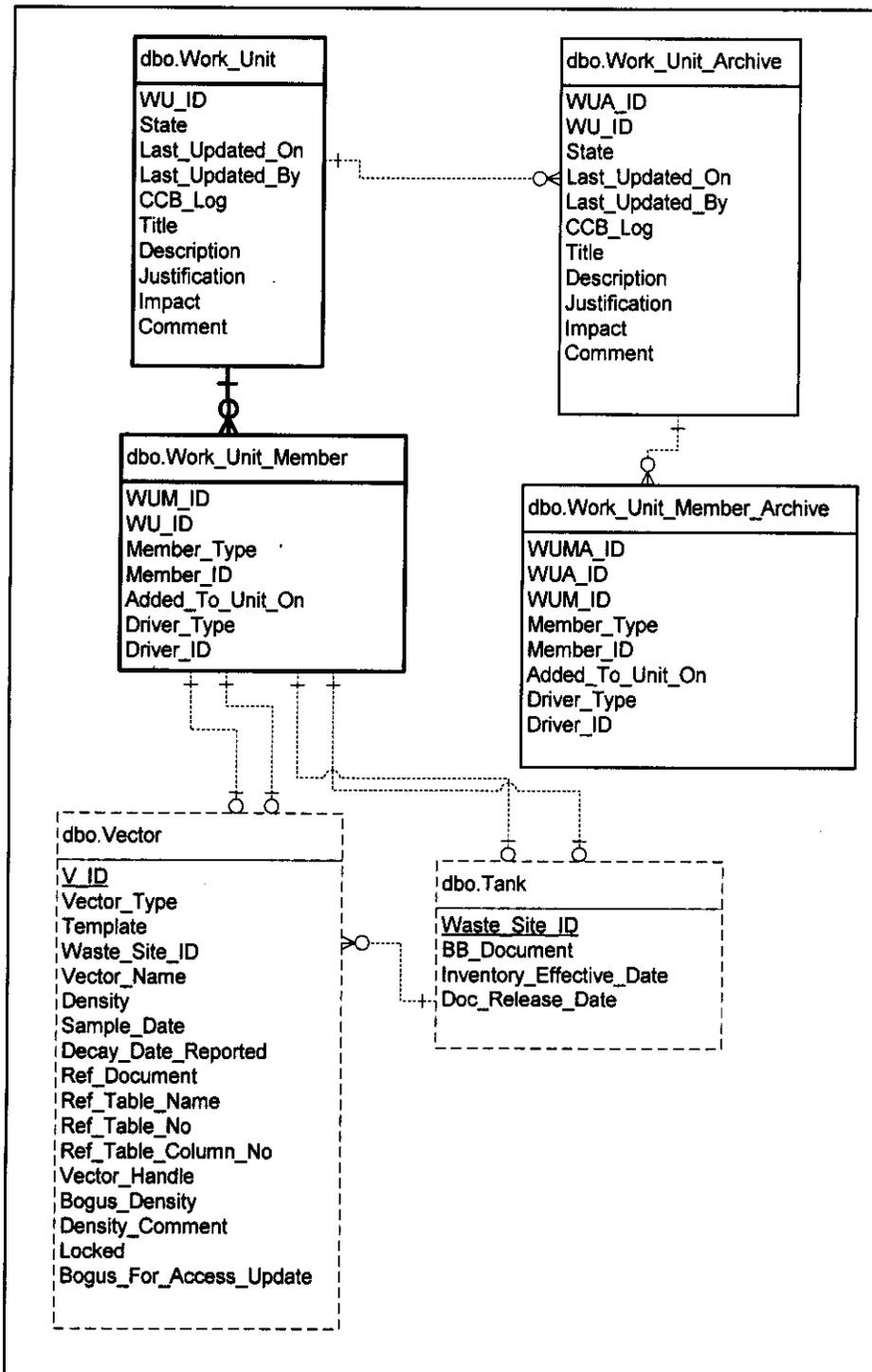
OH_Inventory (in kg) = Net_Charge * Molecular_Weight(OH)/1000

Note: Molecular_Weight(OH) = 17.0017 g

7.9 CONFIGURATION MANAGEMENT

This last section of this chapter discusses the data tables used by the CONFIGMGNT Access program (see Figure 7-6), so that it can be understood more easily.

Figure 7-6. Configuration Management Tools



Any time the **Work_Unit** table or the **Work_Unit_Member** table is changed, the **Work_Unit_Archive** and/or the **Work_Unit_Member_Archive** are used to save the original copy of modified records.

The **Work_Unit** table identifies items in the work area that are at least under consideration for change control. Theoretically, the *State* of the Work Unit determines whether its components are locked, and, thus, cannot be changed by others. But in actual practice, each *Vector* record has a *Locked* field that is checked by the BBIM database before a change is made. If the *Locked* field is set equal to *True*, then the vector cannot be changed. When a user changes the *State* of the Work Unit to *Locked*, the BBIM database will track down all of the vectors associated with the work unit, and set their *Locked* flag equal to *True*. Likewise, when a **Work_Unit** is *Published*, the BBIM database will track down the associated vectors, and set their *Locked* flag equal to *False*.

A Work Unit consists of one more **Work Unit Members**. The **Member_Type** is either *Vector* or *Tank*. The **Member_ID** is either the **Waste_Site_ID** (tank number) or **V_ID** (vector ID).

Currently, the BBIM work area is managed by *Tank*. This allows the users to change vectors as they will. The final results, the tank results, are still protected and cannot be published until the work unit releases them.

If a vector becomes a member of a work unit, all affected tanks must be also become members of the same work unit. In this case, the vector is said to be a **Driver** of the tank. The only kind of **Driver_Type** recognized by the BBIM database is a *Vector*, and the **Driver_ID** is the vector id (**V_ID**).

8.0 REFERENCES

Agnew, S. F., J. Boyer, R. A. Corbin, T. B. Duran, J. R. Fitzpatrick, K. A. Jurgensen, T. P. Ortiz, and B. L. Young, 1997, *Hanford Tank Chemical and Radionuclide Inventories: HDW Model Rev. 4*, LA-UR-96-3860, Los Alamos National Laboratory, Los Alamos, New Mexico.

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A.0 APPENDIX A: DEFINITION OF TERMS

Analyte

Constituent (see definition below).

AvgMult

AvgMult is the abbreviation used on several reports to denote a multiplier used for an Average Vector. It is equal to the average of the different *Mult* values in the Sample Vectors.

AvgRho

AvgRho is the abbreviation used on several reports to denote the density used for an Average Vector. It is equal to the average of the different density values in the Sample Vectors.

Basis

The BBIM database application records the **basis** for each estimate in the inventory. (The inventory might be for a specific phase, or for the total tank). The **basis** is determined by the **vector type(s)** that provided the estimate for the constituent(s). If only one type of vector was used, the following codes apply:

- “E” - all vectors came from process knowledge (Estimated)
- “M” - all vectors came from HDW (Model)
- “S” - all vectors came from Sample Analysis
- “C” - constituent concentrations were Calculated (as explained later)

If an inventory was derived from different vector types, the basis is described by combining the letters for the vector type. For example, if Sample vectors and Model vectors were both used to calculate the inventory of Aluminum, the basis would be shown as “S/M”.

If a constituent is calculated (“C”), it is typically a radioactive isotope. A calculated result will always have a basis of “C” and never anything else.

BBIM

The Best-Basis Inventory Maintenance Tool is a **BBIM database application** used to estimate the amount and content (inventory) of waste stored within waste tanks at Hanford. This term is sometimes used to mean the **BBIM database application** as described below.

BBIM Database

The database portion of the **BBIM database application**. This term is sometimes used synonymously (and probably incorrectly) with **BBIM, BBIM System, BBIM Tool, and BBIM database application**.

BBIM Database Application

As this term implies, the BBIM software application is more than just a database, because a considerable amount of computing is performed to arrive at the estimated inventory.

BBIM System

The people and computers that develop, support, and present the **Best-Basis Inventory**.

BBIM Tool

The **BBIM database application**.

Best-Basis Inventory

The best official estimate of the amount and makeup of the waste stored within Hanford's waste tanks.

Bulk

Inventory can be reported for each waste component, or for the entire tank. An inventory across the entire tank is called a "**bulk**" inventory. This term shows up in some of the BBIM database reports.

CCB Log #

The number assigned to each set of best-basis inventory change records. This number is used to track the changes through the review, approval, and data loading process.

Component (Waste Component)

A **waste component** is a category of waste in the same tank that consists of a single phase of material, which has an estimated or assigned chemical makeup. Each **waste phase** within a tank consists of one or more **waste components**. For example, a batch of slurry from PUREX might be identified as a **waste component**.

Concentration

The amount of constituent per some unit of material (i.e., waste). The BBIM application accepts concentration values in several different formats.

For solid units of concentration (e.g., micro-grams/gram or Curies/gram)

$$\text{Inventory} = \text{concentration} * \text{density} * \text{volume}$$

For liquid units of concentration (e.g., micro-grams/liter or Curies/liter)

$$\text{Inventory} = \text{concentration} * \text{volume}$$

For molar units of concentration (e.g., micro-grams/mole or Curies/mole)

$$\text{Inventory} = \text{concentration} * \text{molecular-weight} * \text{volume}$$

Constituent

Tank waste is analyzed to determine the concentration of many different substances. These substances are often called **analytes** or **constituents**. For example, waste might be analyzed to determine the concentration of aluminum. When this happens, aluminum is said to be a **constituent**. The term **analyte** is not in the dictionary, so often the word **constituent** is used in its place. The two are often used interchangeably.

Density

Density is weight divided by volume. In some of the BBIM reports, density units are not shown, in which case standard units of grams/ milliliter are implied.

Effective Date

The date when the latest BBIM inventory has been effectively agreed upon, but is awaiting approval before it is published for review by the public. Once an inventory estimate is completed, the estimate must be reviewed before it is made official. The **Publish Date** is the day when the inventory is made official. The **Publish Date** follows the **Effective Date**. Different constituents within a tank can have different effective dates.

HDW

Hanford Defined Waste model. Normally, this refers to the latest release of this model data set, which at the time of this writing is HDW Rev. 4.

Inventory

The amount (usually expressed in weight units or Curies) of a tank waste constituent.

Phase (or Waste Phase)

Typical **phases** within a Hanford tank include; supernatant (liquid), saltcake, and sludge.

Publish Date

Once an inventory estimate is completed, the estimate must be reviewed before it is made official. The **Publish Date** is the day when the inventory is made official. The **Publish Date** follows the **Effective Date**.

Representative Vectors

Each time a **waste component** uses a **vector**, a **representative vector** is created to identify the relationship. The **representative vector** mostly is used to store the vector multiplier, but it also allows a vector to be shared by several tanks by creating a new **representative vector** (and multiplier) each time a vector is used or reused. **Representative Vectors** are mostly created for the benefit of the computer and are not important to users. However, one of the BBIM reports lists each **Representative Vector** on the system – thus showing each tank/vector relationship.

Rho

Density -- Rho is a Greek letter that commonly denotes a density variable. When the BBIM tool spells out formulas used to compute analytic inventories, **rho** denotes density.

Standard Decay Date

All radionuclide inventories are automatically decayed by the BBIM database to a certain “standard” date, currently January 1, 1994.

Tank Waste Component

See **Component**.

Tank Waste Phase

See **Phase**.

Tank Waste Type

Tank Waste Type is a name (identifier) for a Waste Component. Two waste components can be given the same name as long as they are either in separate phases or separate tanks from each other.

If a constituent is calculated (“C”), it is typically a radioactive isotope. A calculated result will always have a basis of “C” and never anything else.

Total/Aggregate Waste Phase

See **Total Waste Phase**.

Total Waste Phase

The **Total Waste Phase** is a special phase that applies to the total tank. If the inventory for a constituent (other than hydroxide) is defined in the **Total Waste Phase**, it “overrides” all other inventory calculations in the tank for that constituent. When this happens, the inventory for the constituent (in that tank) is computed from the **Total Waste Phase** rather than summing the inventory from all the different waste components.

V_ID

A numerical identifier that is created and used by the computer to identify a vector. Only programmers typically use this number.

Vector

A collection of one or more constituent concentrations and a density value. Vectors allow the BBIM application to trace lists of estimated concentrations back to their source document.

Vector Basis

See **Vector Type** or **Basis**

Vector Handle

The **Vector Handle** is essentially the short name for the vector. The vector handle string is concatenated from several variables and put together in a string by BBIMCOMBO. The first part of the handle is either an S (sampled data), H (HDW model data), or P (process knowledge). The second part of the string is an abbreviated tank name, and the last part is a serial number, in case a tank has more than one vector associated with it.

Vector Name

Vector_Name is essentially the long name for the vector. Users assign it during data entry. The **Vector_Name** need not be unique, and often isn't.

Vector Type

The **Vector Type** identifies the type of origin (or basis) of the numbers in the vector. A vector is one of the following types:

Sample – Numbers came from sample analysis of the waste

HDW – Numbers came from HDW (a model)

Process Knowledge (see below).

Average (see below)

Process Knowledge vectors are typically generated for waste that comes from a known process. For example, if a batch of waste came from PUREX and went into a tank and was well characterized, BBIM might use that knowledge to build up a vector describing the composition of that waste type.

An “average vector” or “virtual vector” cannot be created directly. Averaging two or more other vectors creates it. Typically an average vector is created when several sample vectors exist for the same waste component, and it is desirable to average their values together to get the best estimate possible. Because an average vector is almost always created from sample data, it is typically of type Sample.

Template Waste Types

“Template” Waste Types are pre-defined waste types that are typically re-used many times. Changing a template, or changing a vector that was used to create a template, can have an impact on many different tanks. Consequently, the BBIM tool provides the ability to assess the impact of making a change to a vector.

Waste Component

See Component.

Waste Phase

See Phase.

Waste Type

See Tank Waste Type.

Work Unit

An official documented change request to the inventory is called a work unit. It is assigned a CCB Log Number.

Work State

A work unit can be in one of several states:

- **Locked** The data of interest are locked, and cannot be changed until they are unlocked.
- **Unlocked** The data of interest can be changed, but the change is not complete yet.
- **Pending** The data of interest have been changed, but are awaiting approval before they are official (published).
- **Published** The change is now official, and released to the public.

WU_ID

An ID that is assigned to a work unit by the computer. The ID is used by the computer and generally will not be of interest to users.

WUA_ID

An ID that is assigned to a Work Unit/Work State by the computer. The ID is used by the computer and generally will not be of interest to users.

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B.0 APPENDIX B: COMPUTATIONAL RULES AND FORMULAE

In the BBIM, computations are done on two levels: first on the component level, and finally on the total tank level. The following two sections break out the calculations in this way.

B1.0 COMPONENT-LEVEL INVENTORY CALCULATIONS:**B1.1 Converting Concentration to Mass (or Curies)**

For solid units of concentration (e.g., micro-grams/gram or Curies/gram or wt%):

$$\text{Inventory} = \text{concentration} * \text{density} * \text{volume}$$

For liquid units of concentration (e.g., micro-grams/liter or Curies/liter):

$$\text{Inventory} = \text{concentration} * \text{volume}$$

For molar units of concentration (e.g., mole/liter):

$$\text{Inventory} = \text{concentration} * \text{molecular-weight} * \text{volume}$$

B1.2 Conversion of Reported Concentration to Standard Concentration:

For Radionuclides:

$$\text{Reported Concentration} \rightarrow \text{Decayed Concentration} \rightarrow \text{Standard}$$

(i.e., the Reported Concentration is first decayed, and then converted to Standard Concentration (uCi/g))

For Chemicals:

$$\text{Reported Concentration} \rightarrow \text{Standard Concentration (ug/g)}$$

(i.e., the Reported Concentration is immediately converted to Standard Concentration (ug/g))

B1.3 Decay Calculations:**Lambda:**

$$\text{Lambda} = \log(2)/(\text{Half_Life_Seconds}/86400)$$

For first order decay:

$$\text{Decay_Factor} = e^{**}(-\text{Lambda} * \text{Ndays})$$

For second order decay:**For each daughter in Decay_Chain**

$$\text{Second_Order_Decay_Factor} = (\text{Decay_Factor_of_daughter} + ((\text{Daughter.Lambda})/(\text{daughter.lamda-parent.lamda})) * (\text{Parent_Decay_Factor} - \text{Daughter_Decay_Factor}))$$

$$\text{Decayed_Concentration} = \text{Rpt_Concentration} * \text{Decay_Factor}$$

B1.4 Dependent Constituents (Ratios)**FOR a Dependent Constituent (one that is found in the Constituent_Dependent Table)****IF (a non-calculated inventory number does not exist for constituent1) THEN****IF (an inventory number does exist for constituent 2) THEN**

$$\text{Constituent1_Inventory} = \text{Constituent2_Inventory} * \text{Constituent_Dependents.Factor}$$

B1.5 Computing Concentrations from HDW Model Ratios.**Inv_Con**

This constituent is listed in the first column of the **U_and_Pu_Dependents** table. The amount of inventory for **Inv_Con** must be stored in the **Tank_Waste_Inventory** table, and it must come from Sampling information or from Process Knowledge.

It is assumed that BBIM will not contain sampled and/or process knowledge values for both *Pu239* and *Pu239/Pu240* in the same vector. If this happens, Pu-239/Pu-240 values take precedence.

HDW_Con:

This constituent is listed in the second column of the **U_and_Pu_Dependents** Table and is used when the **Tank_Waste_Inventory** table does not have a non-calculated inventory value stored for this constituent.

FOR EACH RECORD IN U_and_Pu_Dependents Table

FOR EACH useable Inv_Con entry (see above)

FOR EACH useable HDW_Con entry (see above)

$$\text{HDW_Con.value} = \text{Inv_Con.value} * \text{HDW_Con.Model} / \text{Inv_Con.Model}$$

(Value = final estimated inventory value.

Model = inventory estimated in the HDW Model.)

B1.6 Average Vector Factors

IF Average_Vector_Is_Created THEN

Average_Vector_Density = average of the component vector densities

Average_Vector_Multiplier = average of the component vector multipliers

B1.7 Computing Inventory of Hydroxide.

FOR EACH constituent in the waste component (also includes Total component)

IF the constituent is not in a Locked state in CONFIGMGNT

$$\text{Net_Charge} = \text{Net_Charge} \\ + \text{BBIM_inventory (in kg)} * 1000 * \text{primary_valence_count} / \text{Molecular_Weight}$$

ELSE use the Locked value which is in BB_Published

$$\text{Net_Charge} = \text{Net_Charge} \\ + \text{BB_Published_inventory (in kg)} * 1000 * \text{primary_valence_count} / \text{Molecular_Weight}$$

$$\text{OH_Inventory (in kg)} = \text{Net_Charge} * \text{Molecular_Weight(OH)} / 1000$$

Note: Molecular_Weight(OH) = 17.0017 g

B2.0 TOTAL TANK-LEVEL INVENTORY CALCULATIONS:

B2.1 Summing Inventory of Each Tank Component to Get Total Inventory:

```
FOR EACH tank,  
  FOR EACH constituent_in_the_tank  
    IF constituent_is_a_component_of_the_“Total_Phase” THEN  
      Tank_inventory_of_that_constituent =  
        The_inventory_of_that_constituent_in_the_”Total_Phase”  
    ELSE (constituent isn’t listed as part of the “Total_Phase”) THEN  
      Tank_inventory_of_that_constituent =  
        Sum_of_inventories_across_each_tank_component.
```

B2.2 Computing Inventory from Total Alpha (Across the Entire Tank)

```
If we have a Total_Alpha measurement for the tank then  
HDW_List = List of constituents tracked in the model that produce alpha  
All_HDW_List = Sum of HDW Alpha for each constituent in HDW_List  
All_Tank_Alpha = Total Alpha measurement for the tank  
Tank_List = List of all constituents in the HDW_List that we have  
estimates for, that do not come from a model or from a  
previous Total Alpha estimate.  
Work_List = List of all constituents that are in HDW_List but not  
Tank_List  
  
FOR EACH constituent in Work_List  
  Inventory = HDW_Estimate * All_Tank_Alpha/All_HDW_Alpha
```

B3.0 DEFAULT BASIS SELECTION ALGORITHM:

B3.1 1. Initialize Basis Button on Radio Button Form:

When BBIM radio button form Initialize Basis button is pressed, the form uses the following algorithm to select a constituent concentration from among several vectors:

For each Constituent, select in the following order of preference:

If possible, use a Sample (S) vector from the same tank, but don't select S vectors from another tank and don't select multiple S vectors from the same tank.

Use an E (Sample Average vector group) vector for waste type in this tank

Use a P (Process Knowledge) vector.

Use a M (Model) vector.

If the Qualifier for a constituent is NR or NA, use the next most preferable vector for that constituent.

'<' values are acceptable. In the case of two choices, one of which is a <, use the lowest value.

C.0 APPENDIX C - DATA MODEL DIAGRAMS

Figure C-1. Main Data Tables for BBIM

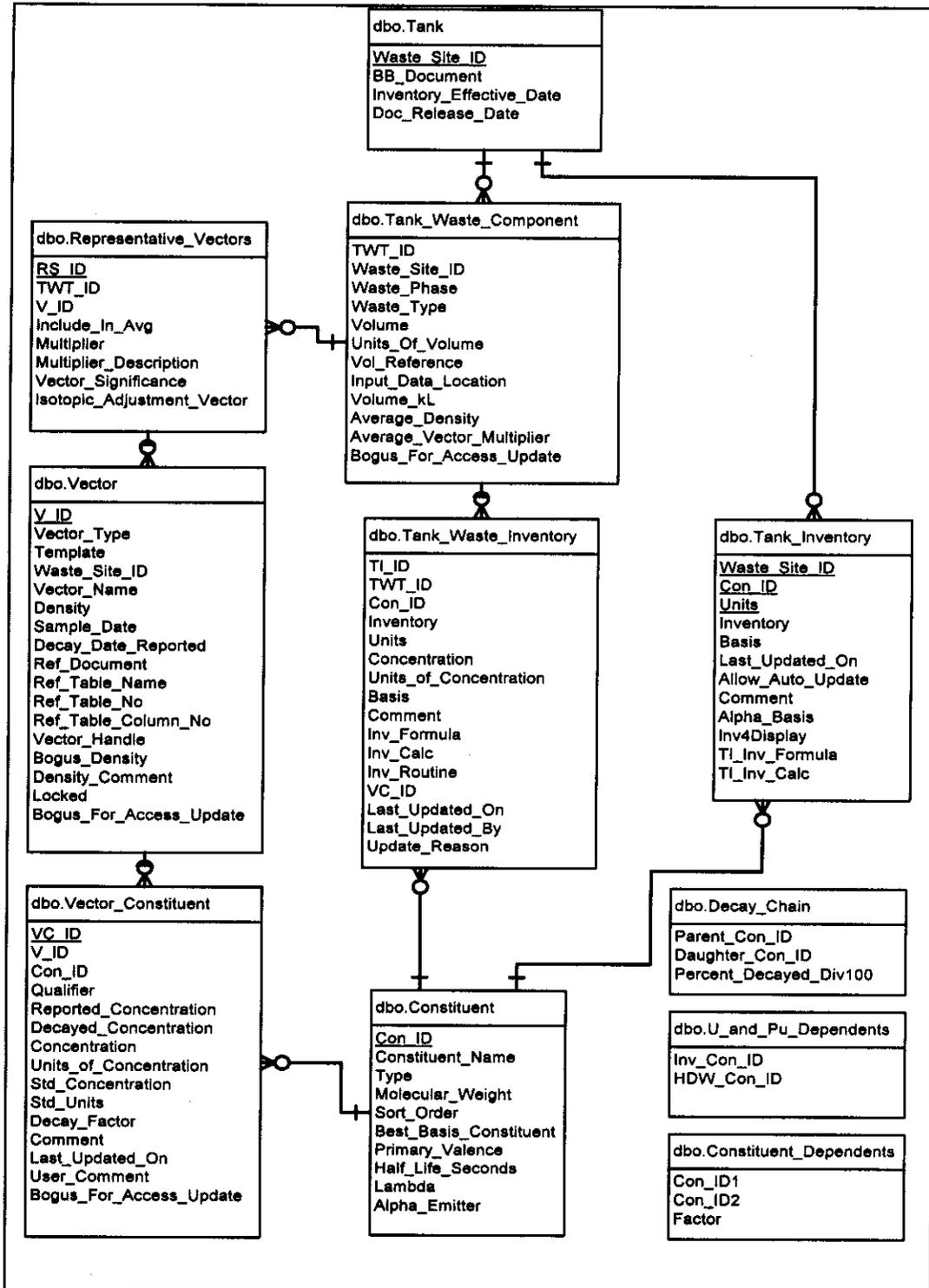


Figure C-2. Configuration Management Data Model Extensions (dashed boxes)

