1/29

PRETREAT: A SPREADSHEET-BASED MASS-BALANCE MODEL FOR HANFORD TANK WASTE REMEDIATION SYSTEM PRETREATMENT PROCESSES

Prepared for

Nuclear Regulatory Commission
Contract NRC–02–97–009

Prepared by

Lietai Yang
Roberto T. Pabalan

August 2000

2/29

CONTENTS

FIGURES

4/29

TABLE

ACKNOWLEDGMENTS

This report was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the Nuclear Regulatory Commission (NRC) under Contract No. NRC-02-97-009. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of Fuel Cycle Safety and Safeguards. This report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

The authors gratefully acknowledge the assistance of A. Ramos in the preparation of the manuscript, V. Jain for technical review, B. Sagar for programmatic review, and the NRC staff for their comments and suggestions.

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: This report contains no CNWRA-generated laboratory or field data. Sources of data are referenced within the report. Data from these sources are used freely, and these sources should be consulted for determining the level of quality for those data.

ANALYSES AND CODES: The spreadsheet model PRETREAT Version 0 was developed using the software Microsoft Excel 97. This software is a commercial code and only the object code is available to the CNWRA. The Excel file Pretreat.xls that contains the working model will be maintained with the Quality Assurance records for this report. Following NRC acceptance, PRETREAT Version 0 or later versions will be placed under CNWRA configuration control. Information on the development of PRETREAT Version 0 can be found in CNWRA Scientific Notebook Number 352.

1 INTRODUCTION

1.1 BACKGROUND[1]

The U.S. Department of Energy (DOE) is legally bound to remediate the 204,000 m^3 (54 million gal.) of high-level radioactive waste (HLW) stored in 177 aging underground storage tanks at the Hanford site. Under the Tank Waste Remediation System (TWRS) program, the current plan for remediating these wastes consists of waste retrieval, pretreatment, immobilization, and disposal. Because of the expected high cost of HLW vitrification and geologic disposal, the retrieved waste will be chemically separated to form a HLW stream, which will contain most of the radionuclides, and a low-activity waste (LAW) stream, which will contain the bulk of the nonradioactive chemicals and the soluble components of the tank waste. The HLW stream will be vitrified and the product stored until it can be transferred to a licensed HLW geologic repository. The LAW stream, after removal of cesium, strontium, technetium, and transuranic elements, will be solidified in a glass form also, but will be stored at an onsite retrievable disposal facility. The radionuclide concentrations in the immobilized LAW are required to meet the Nuclear Regulatory Commission (NRC) Class C limits. To meet these limits, pretreatment of the LAW stream is required to remove cesium-137, strontium-90, technetium-99, and transuranic elements from the waste feed. Removal of nonradioactive elements that could significantly increase the volume of immobilized LAW, such as sodium, or deleteriously affect vitrification of the wastes, such as sulfur, may also be necessary.

The DOE has chosen to privatize the construction and operation of the TWRS [i.e., the DOE had planned to use a contractor-owned and contractor-operated (COCO) facility, rather than the more common (for the DOE) government-owned and contractor-operated (GOCO) facility, to accomplish this task]. The Tank Waste Remediation Systems Privatization (TWRS-P) program has been divided into two phases: Phase I, with Parts A and B, is the proof-of-concept or demonstration phase, and Phase II is the full-scale operations phase. The DOE completed Part A of Phase I, which consisted of a feasibility study, in fiscal year (FY) 1998, and awarded a contractor team led by BNFL Inc. to proceed to Part B-1 of Phase I of the TWRS-P project. Phase I/Part B-1 is a 24-mo design period during which BNFL Inc. will address technology scale-up; regulatory, financial, and permitting issues; and the safety basis for operations. At the conclusion of this period, the DOE will make a decision whether to proceed with BNFL Inc. into the construction and operations phase (Phase I/Part B-2).

If authorized to proceed to Phase I/Part B-2, BNFL Inc. will provide both HLW and LAW treatment and immobilization services. During Phase I/Part B-2, BNFL Inc. will begin waste pretreatment in 2005, HLW vitrification in 2006, and LAW vitrification in 2007. During vitrification operations from 2006 through 2018, the contractor is expected to process approximately 10 percent of the Hanford tank waste by mass and 20–25 percent by radioactivity. After Phase I/Part B-2 operations, the DOE will decide to either deactivate the facility or use it for Phase II waste processing. The DOE plans to issue a new procurement for Phase II in FY2010 for processing the remainder of the tank waste using the existing facility or a new facility of similar size and capacity.

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[1]The discussion presented in this section is based on information that was publicly available as of January 15, 2000. Subsequent to completion of this report, the DOE has terminated its privatization contract with BNFL Inc. The DOE plans to issue a request for proposals for design and construction of a Hanford waste treatment facility in August 2000, and to select a replacement contractor by January 15, 2001 (http://www.hanford.gov/press/2000/orp/062900.orp.html).

Phase II facilities may be subject to NRC licensing and regulation. A Memorandum of Understanding between the DOE and the NRC (U.S. Department of Energy/Nuclear Regulatory Commission, 1997) was prepared under which the NRC involvement in Phase I activities has three objectives: (i) acquire sufficient knowledge of the physical and operational situation at the Hanford waste tanks, (ii) assist DOE in performing reviews in a manner consistent with the NRC regulatory approach, and (iii) be prepared to develop an effective regulatory program for the possible licensing of DOE COCO facilities. The Center for Nuclear Waste Regulatory Analyses (CNWRA) has been engaged by the NRC to assist in developing the technical and regulatory tools for the TWRS-P. A broad objective of the CNWRA activities is to provide NRC staff with information and tools needed to assess the chemical, radiological, and criticality hazards of Hanford tank wastes and TWRS-P operations.

An overview of the TWRS program and a review of the pretreatment technologies proposed by BNFL Inc. to process the Hanford tank wastes were presented previously (Pabalan et al., 1999). The DOE will provide tank waste to BNFL Inc. that includes three LAW feed types (i.e., envelopes A, B, and C wastes). A fourth waste type (envelope D waste) would consist of the double-shell tank sludges. The four waste types are representative of the range of Hanford tank wastes. Envelopes A, B, and C wastes contain cesium-137 and technetium-99 at concentrations that make their removal necessary to ensure that the LAW glass specification can be met. Envelope B waste contains higher concentrations of cesium-137 than envelopes A and C wastes, as well as higher concentrations of chlorine, chromium, fluorine, phosphates, and sulfates, which may limit the waste loading in the glass. Envelope C waste contains organically complexed strontium-90 and transuranic elements that will require removal. Envelope D waste contains an HLW slurry. The pretreatment process, which will prepare the radioactive wastes into a stream with a suitable chemical composition for vitrification, involves several unit operations including evaporation, precipitation, filtration, and ion exchange.

Important considerations in the evaluation of the BNFL Inc. pretreatment flowsheet are radiological and chemical safety, as well as the effectiveness of the proposed pretreatment technologies. Assessments of potential radiological and chemical hazards and the strategies for mitigating these hazards require a knowledge of the chemical compositions and radionuclide concentrations of the low-activity and high-activity waste streams at each stage of the pretreatment process. For example, the concentrations of gamma-emitting radioisotopes in process equipment will determine shielding requirements for the equipment. Radioactive decay heat from radioisotopes could increase the waste temperature and influence the moisture loss rate (e.g., in waste feed tanks) and could accelerate degradation of ion exchange resins. The concentrations of radionuclides, as well as those of chemical components that affect waste loading (e.g., sodium and sulfate), at the end of the pretreatment process will determine whether the LAW can be immobilized in a glass form that will meet NRC Class C limits. Evaluation of potential criticality in the pretreatment facility (e.g., in the transuranic ferric flocculation/precipitation process) requires information on the concentration of fissile materials. For organic-bearing wastes, a knowledge of the concentrations of organic complexants would help in evaluating the potential for hydrogen gas generation, organic exothermic reactions, and reduced efficiency of pretreatment methods (e.g., ferric flocculation/precipitation) due to organic complexation of radionuclides.

A mass-balance model could provide an ideal tool for this purpose. Commercial simulation software packages such as Aspen Plus (Aspen Technology, Inc., Cambridge, Massachusetts), PRO/II (Simulation Science, Inc., Brea, California), HYSIM (Hyprotech, Inc., Calgary, Alberta, Canada), and OLI ESP (OLI Systems, Inc., Morris Plains, New Jersey) have been widely used in thermodynamic simulations of many industrial chemical processes. These software packages not only calculate mass balances but also energy balances using thermodynamic parameters stored in databases. Some of the software permit dynamic simulations and calculations of process stream properties as a function of time. However, these software packages are subject to some or all of the following limitations:

(i) Long simulation times. The Hanford wastes are extremely complex and may contain hundreds to thousands of chemical species, which makes chemical simulations prohibitively long for some software packages.

(ii) Lack of support for radioactivity calculations and lack of thermodynamic data for some species found in Hanford wastes.

(iii) Difficulty in simultaneously considering all the unit operations proposed for the Hanford pretreatment flowsheet. Some of the pretreatment unit operations, such as filtration, ion exchange, and the melter, are not supported by the commercial software packages.

1.2 OBJECTIVE

To provide the NRC with a tool that can aid in evaluating the chemical, radiological, and criticality hazards of the TWRS-P, a Microsoft Excel© spreadsheet model—PRETREAT Version 0—of the BNFL Inc. flowsheet was developed. The model is based on mass-balance considerations and user-specified waste feed envelope compositions and concentration factors (e.g., from evaporation) or decontamination factors (e.g., by ion exchange or ferric flocculation/coprecipitation). However, compared with commercial software packages, PRETREAT does not support thermodynamic calculations.

Applications of PRETREAT include estimating radionuclide and chemical species concentrations in the waste stream at each stage of the pretreatment process and estimating the amount of spent ion exchange resin or the amount of secondary wastes generated by the pretreatment process. The model can also be used to evaluate the effects of uncertainties in model parameters (e.g., the decontamination factors), for example, on the potential for noncompliance with NRC Class C limits of the immobilized LAW. This document describes the use and the technical basis of the model.

2 TECHNICAL BASIS

2.1 PROCESS FLOWSHEET[2]

Figure 2-1 shows a flow diagram of PRETREAT. The numbers in figure 2-1 correspond to the process units or waste streams listed in table 2-1. Figure 2-1 represents the BNFL Inc. flowsheet described in Calloway et al. (2000), with the exception of the Auxiliary Input Streams and the Feed unit. The use of the Auxiliary Input Streams in the model for some process units allows the flexibility to analyze the subsequent unit(s) with an additional input that may not have been anticipated during the development of PRETREAT. The Auxiliary Input Streams can also be used to analyze the subsequent unit(s) as stand-alone unit(s) by setting the incoming stream from a preceding unit to zero flow. The ability to treat certain units in a stand-alone mode may facilitate analyses of the behavior of the hazardous materials in that unit.

The Feed unit in the BNFL Inc. design is part of the LAW Evaporation unit. PRETREAT handles the Feed section as a separate unit for convenience.

The process flowsheet consists of the six operational units described in the following sections.

2.1.1 Low-Activity Waste Evaporation

This unit removes excess water in the waste to reduce the burden on the rest of the pretreatment units. The sodium concentration in the evaporator concentrate (Stream 14) is controlled at about 7 M. The evaporator overhead is condensed, collected, and used as wash water in the various units of the plant.

2.1.2 Precipitation/Ultrafiltration

This unit removes the solids and precipitates from the liquid LAW. The precipitation treatment in this unit is only applied when the LAW contains Type C feed, which contains complexing agents that hinder the precipitation of strontium-90 and transuranic elements. To meet the contract-specified radionuclide concentration limits for the immobilized LAW (20 Ci/m^3 for strontium and 100 nCi/g for transuranic elements), the concentrations of strontium-90 and transuranic elements in the LAW must be reduced. The concentrated slurry (Stream 24) is either sent to the DOE, if BNFL Inc. is contracted to treat the LAW only, or sent to the HLW vitrification system, if BNFL Inc. is contracted to treat both HLW and LAW (the HLW vitrification system is not represented in PRETREAT).

2.1.3 Cs Ion Exchange

The cesium ion exchange unit is designed to reduce the cesium content in the LAW so that the cesium-137 content of the waste glass complies with the contract-specified limit of 3 Ci/m^3.

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[2]The discussion of the BNFL Inc. flowsheet is based on information that was publicly available as of January 15, 2000. Subsequent to completion of this report, the DOE has terminated its privatization contract with BNFL Inc. The DOE plans to select a replacement contractor by January 15, 2001 (http://www.hanford.gov/press/2000/orp/062900.orp.html). Changes to the process flowsheet may be implemented by the new contractor.

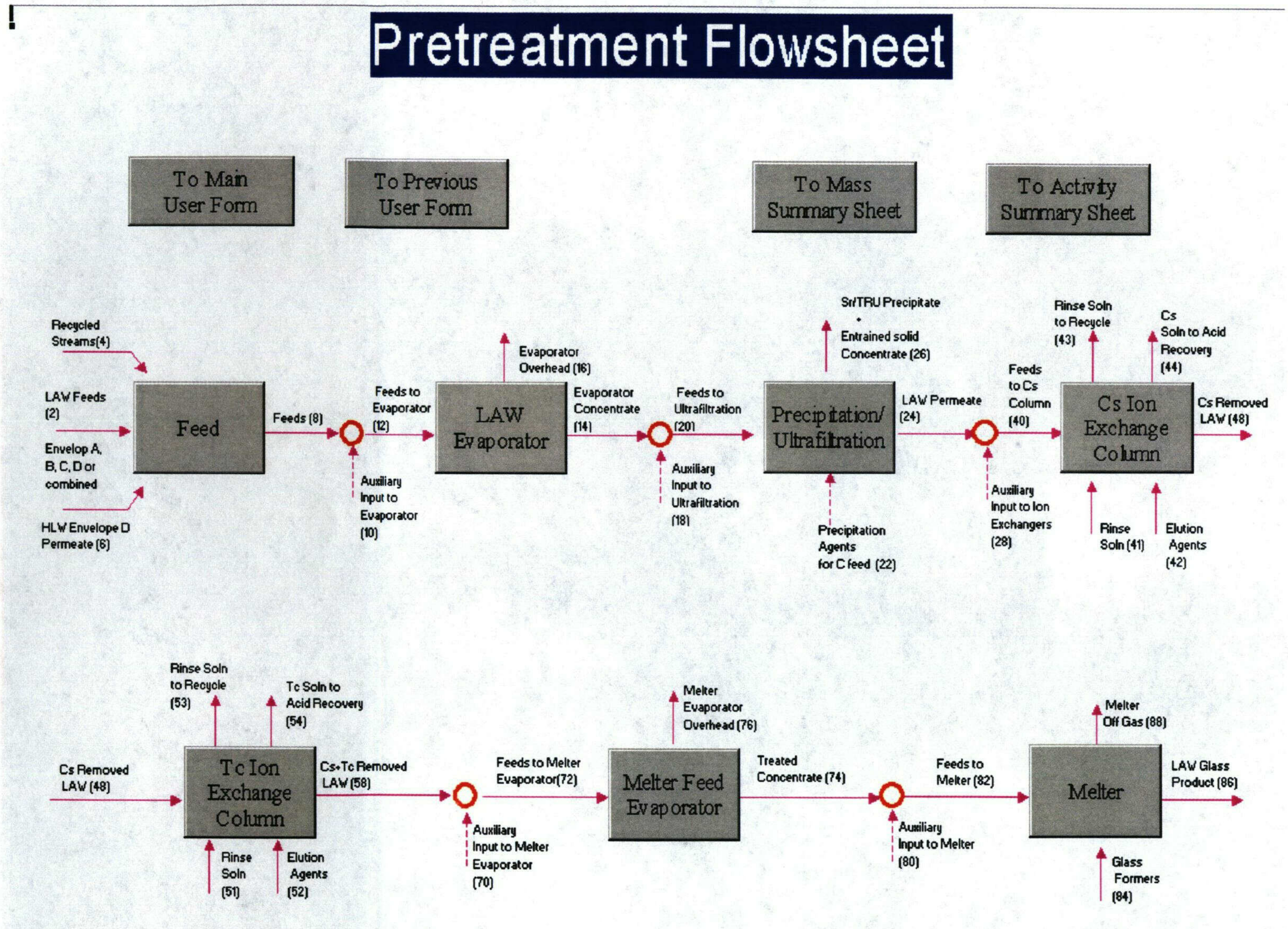


Figure 2-1. PRETREAT flow diagram representation of the BNFL Inc. pretreatment process flowsheet

10/25

Table 2-1. List of PRETREAT flowsheet process stream numbers and corresponding process units and stream names

Process Units	Process Stream Numbers	Process Stream Names	Remarks
	2	LAW Feed	Envelope A, B, C, D feeds from DOE
	4	Recycled Stream	comes from the plant
	6	HLW Envelope D Permeate	comes from the pretreatment plant
	8	Feed	feed to the pretreatment plant
LAW Evaporator	10	Auxiliary Input to Evaporator Unit	added for modeling and analysis purposes
	12	Feed to Evaporator	same as #8 if #10 is set to zero
	14	Evaporator Concentrate	feed to ultrafiltration
	16	Evaporator Overhead	to be used as process wash water
Precipitation/Ultrafiltration	18	Auxiliary Input to Ultrafiltration	added for modeling and analysis purposes
	20	Feed to Ultrafiltration	same as #14 if #18 is set to zero
	22	Precipitation Agents and Wash Water	NaOH, $Fe(NO_3)_3$, $Sr(NO_3)_2$, HNO_3, and H_2O
	24	LAW Permeate	feed to Cs column
	26	Sr/TRU Precipitate & Entrained Solid Concentrate	in slurry form, with about 50 volume percent solids
Cs Ion Exchange Column*	28	Auxiliary Input to Ion Exchanger Columns	added for modeling and analysis purposes
	40	Feed to Cs Column	same as #24 if #28 is set to zero
	41	Rinse Solution	NaOH solution and water
	42	Elution Agents	HNO_3 solution and water
	43	Rinse Solution to Recycle	to Stream 4 (including regeneration solution)
	44	Cs Solution to Acid Recovery	to acid recovery system; the recovered acid to be reused in Stream 42
	48	Cs Removed LAW	Cs-free LAW solution

Table 2-1. List of PRETREAT flowsheet process stream numbers and corresponding process units and stream names (cont'd.)

Process Units	Process Stream Numbers	Process Stream Names	Remarks
Tc Ion Exchange Column*	48	Cs Removed LAW	Cs-free LAW solution
	51	Rinse Solution	NaOH and water
	52	Elution Agents	HNO_3 solution and water
	53	Rinse Solution to Recycle	to Stream #4 (including regeneration solution)
	54	Tc Solution to Acid Recovery	to acid recovery system; the recovered acid to be reused in Stream 52
	58	Cs+Tc Removed LAW	Cs- and Tc-free LAW solution
Melter Feed Evaporation	70	Auxiliary Input to Melter Evaporator	added for modeling and analysis purposes
	72	Feed to Melter Evaporator	same as #58 if #70 is set to zero
	74	Treated Concentrate	ready as feed to the melter
	76	Melter Evaporator Overhead	to be used as process wash water
Melter	80	Auxiliary Input to Melter	added for modeling and analysis purposes
	82	Feed to Melter	same as #74 if #80 is set to zero
	84	Glass Formers	oxides, silicates, and carbonate
	86	LAW Glass Product	immobilized LAW in glass form
	88	Melter Off-Gas	to off-gas treatment processes

*Regeneration solutions are not considered in the mass balance because they are not mixed with the main streams, but are recycled as future rinse solutions.

2.1.4 Tc Ion Exchange

Similar to the cesium ion exchange unit, the technetium ion exchange unit is designed to reduce the technetium content in the LAW so that technetium-99 in the waste glass is below the contract-specified limit 0.3 Ci/m^3.

2.1.5 Melter Feed Evaporator

The melter feed evaporator is designed to further remove excess water in the final feed to the melter unit. The sodium concentration in the final feed to the melter unit will be controlled at about 9 M.

2.1.6 Melter

The LAW and glass-forming materials will be fed to the melter and converted into a glass product. The composition of the glass is adjusted by changing the quantity and the composition of the glass-forming stream (Stream 84). Water and other volatile components in the LAW feed are evaporated into the off-gas stream (Stream 88) and treated before they are vented or discarded into the environment.

2.2 SPREADSHEET CALCULATIONS

The mass-balance model is implemented in a Microsoft Excel (Version 97) spreadsheet environment.

2.2.1 Representation of Waste Streams

Figure 2-2 shows a typical table in PRETREAT with selected components (the full table tracks 57 inorganic elemental and 14 organic components). The stream properties, such as stream name, envelope contents, total mass or volume flow, and density are at the top of the table. Listed in two columns are the concentrations of the waste stream components, expressed in grams per liter (g/L), and the activities of the radionuclides, given in units of becquerels per liter (Bq/L). Listed at the bottom are properties such as total transuranic elements (TRU), total organic carbon (TOC), and fissionable materials (Pu-239/Pu-241 and U-235) in solids. The properties at the bottom of the table are considered to be important to safety. Because these properties have been already included in the sum of the detailed component list, they are placed at the bottom of the table to avoid being counted twice.

2.2.2 Process Units and Their Associated Process Streams

There are seven process units in PRETREAT (feed is treated as a separate unit in the model). The flow diagram for each process unit and the streams (both input and output) associated with the process unit are placed in a single worksheet. Figure 2-3 shows a typical worksheet for one of the process units, the LAW evaporator unit.

There are two command buttons in every worksheet of PRETREAT. The functions of these buttons are discussed in section 3.1.1.

To Main Form

Back to User Form

Stream Name:	LAW Feeds
Stream No:	2
Tot Mass (Mt/d):	**61.9637**
Tot Vol (m3/d):	5.20E+01
Density (Mt/m3):	**1.19161**
Tot Act. (Bq/d):	**6.98E+14**
Temperat. (oC):	2.00E+01
Feed Type:	A

Ionic Comp	g/L
Al	12.0000
B	0.0000
Ba	0.0000
CN	0.0000
C as CO3	0.0000
Ca	0.0000
Cd	0.0000
Cl	3.0000
Cr	0.1799
F	0.0000
Fe	0.0030
H2O	981.5694
Hg	0.0000
K	1.8935
La	0.0000
Li	0.0000
Mg	0.0000
Mn	0.0000
Na	82.0000
Ni	0.0000
NO2	23.4087
NO3	50.9215
OH	5.0000
Pb	0.0000
P as PO4	0.7389
Pu(total)	0.0000
Si	0.0000
S as SO4	1.7374
Sr	0.0000
U (total)	0.0000
Zn	0.0000
Zr	0.0000

Other C	g/L
Precip.	0.1000
Solids	18.3926
TIC	7.5000
TOC	2.9641
CsIX	0.0000
TcIX	0.2000

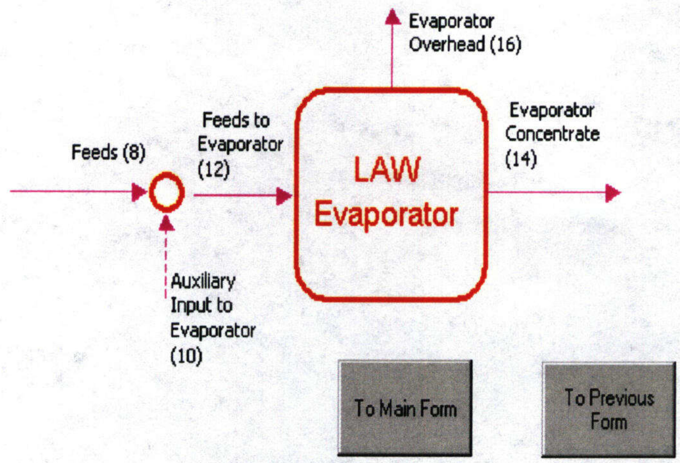
Gases	g/L
CH4	0.0000
H2	0.0000
N2	0.0000
NH3	0.0000
NO	0.0000
NO2(g)	0.0000

Fissile	g/L
Pu239/241	0.00E+00
U-235	0.00E+00

Activity	Bq/m3
Am241	0
Ba137m	0
Co60	1.30E+01
Cs137	1.27E+13
Eu154/155	4.12E+09
Ni63/59	0
Pu	0
Sm151	0
Sr90	1.30E+11
Tc99	2.11E+10
TRU	1.42E+09
Y-90	0
Solid	5.22E+11

Figure 2-2. Example of a table used in PRETREAT listing waste stream properties

15/29



Stream No	12		14		16	
Stream Name	Feeds to LAW Evaporator		LAW Concentrate		Evaporator Overhead	
Stream Temp	20		20		20	
Envelope A (%)	0		0		0	
Envelope B (%)	96		96		96	
Envelope C (%)	4		4		4	
Envelope D (%)	0		0		0	
Mass Flow, g/d	1.7909E+08		8.1099E+07		9.7989E+07	
Volume Flow, L/d	1.7000E+05		7.2025E+04		9.7975E+04	
Density, g/L	1.0535E+03		1.1260E+03		1.0001E+03	
Activity Flow, Bq/d	2.8110E+13		2.8082E+13		2.8110E+10	
Component	**Mass, g/L**	**Ativity, Bq/L**	**Mass, g/L**	**Ativity, Bq/L**	**Mass, g/L**	**Ativity, Bq/L**
INORGANICS						
Ag	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Al	1.0000E-01	0.0000E+00	2.3579E-01	0.0000E+00	1.7351E-04	0.0000E+00
Am/Am241,242	0	1.0000E+07	0	2.3579E+07	0	1.7351E+04
Zr	2.0000E-03	0	4.7159E-03	0	3.4703E-06	0
Others Inorg.	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
ORGANICS						
Acetate	1.0000E-07	0	2.3579E-07	0	1.7351E-10	0
TBP	1.5000E-06	0	3.5369E-06	0	2.6027E-09	0
Other Organics	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
	0	0	0	0	0	0
SUM	1.0535E+03	1.6536E+08	1.1260E+03	3.8990E+08	1.0001E+03	2.8691E+05
Total TRU	0.0000E+00	1.4200E+06	0.0000E+00	3.3483E+06	0.0000E+00	2.4639E+03
TIC	7.5000E+00	0	1.7684E+01	0	1.3014E-02	0
TOC	2.9641E+00	0	6.9891E+00	0	5.1431E-03	0
Total solids	1.8393E+01	5.0000E+07	4.3412E+01	1.1801E+08	0.0000E+00	0.0000E+00
Pu239/241 in solids	0.0000E+00	4.0000E+06	0.0000E+00	9.4411E+06	0.0000E+00	0.0000E+00
U235 in solids	0.0000E+00	3.5000E+05	0.0000E+00	8.2610E+05	0.0000E+00	7.7871E-11

Figure 2-3. Typical worksheet for a process unit (low-activity waste evaporator unit). Only selected components are shown; the actual table tracks more than 70 components).

2.2.3 Calculation for Process Units

Given the flow rates and chemical compositions of the input streams, the properties of the output streams can be calculated based on the process properties and the output requirements. For instance, the amount of strontium going to Stream 24 (see figure 2-1) is dependent on the filtration unit properties, such as filter size and filtering pressure, and strontium properties, such as the solubility and particle size of the strontium precipitate that forms. A reduction or concentration factor (called component factor in the model) is used to represent the overall effect of both the process unit and the component on the distribution of each component among the output streams. The component factor is defined as the ratio of the amount of a component in the main process output stream to the total amount received from the input stream. The input from the service streams, such as the precipitation agent, wash water, or glass-forming agent, are not counted in the total amount received from the input streams.

Among the component factors, only a few are known or can be calculated for the given properties or requirements of a process unit, and their values are estimated during the calculation. Therefore, the user of PRETREAT is allowed to modify the component factors during the modeling process. In addition, the process parameters of certain units, such as the sodium concentration in the feed to the melter, may change from time to time and the user of the model is also allowed to make such changes during the modeling process.

For the filtration and melter units, assays for most of the components in the filter solids and the glass product are readily available during production, thus the component factors for the assayed components are back-calculated from the assay results. The user is required to specify the assay results for those components, instead of the component factors.

A separate calculation worksheet is used for each process unit to contain both the process parameters and the component factors used in the calculations. A portion of a typical calculation sheet is shown in figure 2-4. Intermediate calculations are also performed on this worksheet. The results of the intermediate calculations are normally placed below the component factors table or to the right of the process parameters table. To minimize confusion during routine use, the rows and columns that contain the calculation results are hidden from the user. To view these data, the user can go to the worksheet, highlight the hidden columns or rows (the rows or columns that are missing from the worksheet), choose Row or Column from the format menu bar, then select Unhide.

2.2.4 Independent Input Streams

Independent input streams in PRETREAT are those whose properties are not directly dependent on the Process Parameters of the process units. These streams include

- Envelope Streams (Envelopes A, B, C, and D)
- Feed Streams (Streams 2, 4, and 6) when they are not linked to the envelope streams
- Auxiliary Input Streams (Streams 10, 18, 28, 70, and 80)

The independent input streams usually require specifications from the user during the modeling process. In addition to their appearance on the process unit worksheet, the specifications are also placed on a separate worksheet so they can be specified or modified more easily. When a user modifies data in the separate worksheet, values in the corresponding input streams in the process unit worksheet are automatically updated.

To Main Form | To Previous Form | To Main Form | To Previous Form

Component Factors:

Component Factors:
(Fraction of components that remain in the peameate stream)

Component	Factor
INORGANICS	
Ag	**0.0000**
Al	**1.0000**
Am/Am241,242	0.5020
As	**0.0000**
B	**0.0000**
Ba/Ba137	0.1000
Be	**0.0000**
Bi	**0.0000**
C (as CO3)	**1.0000**
Ca	**0.0000**
Cd	**0.0000**
Ce	**0.0000**
Cl	**0.8615**
CN	**1.0000**
Co/Co60	0.0100
Cr	**0.6545**
Cs/Cs137,134	0.5500
Cu	**0.0000**

Process Parameters:

	Parameters	Values	References/Notes
1	pH prior to NaOH addition	13.2	
	Free OH prior to NaOH addin (M)	**0.158489319**	The OH in the mass balance tables is not free OH
2	OH after 19 M NaOH addition (M)	1	BNFL Report
3	Fe(NO3)3 in Solution after addition (M)	0.075	BNFL Report, 1999. For Envelope C only
4	Sr(NO3)2 in Solution after addition (M)	0.075	
5	Number of Water Wash Cycle	4	
6	Vol of wash water to slurry ratio	1	
7	Density of slurry stream (#24)	**1.136907936**	From Filtration sheet
8	Na in final Slurry (g Na/kg dry solid)	60	BNFL Report, 1999
9	Density of 19 M NaOH solution^	1.515	Aldrich Chemicals Catalog 1998/1999, P1509
10	Fe+++/Fe ratio in Stream 20	0.5	N/A
11	Density of 3.5M Fe(NO3)3 solution^	1.5	N/A
12	Sr++ in Stream 20 (M)	0	
13	Density of 1 M Sr(NO3)2 solution^	1.2	N/A
14	Efficiency of solids removal	99.9	N/A
15	Vol % of solids in slurry	50	
16	Desnsity of solids from feed	2	N/A, assuming zero void
17	% of Sr(OH)2 precipitated	90	N/A
18	Desnsity of precipitated^^	2.6	FeO(OH)=3.5--Alfa Aesar Catalog, P376, assuming zero void
19	O Atomic weight	**16**	
20	H Atomic weight	**1**	
21	Fe Atomic weight	**55.85**	
22	Sr Atomic weight	**87.62**	
23	Na Atomic weight	**22.99**	
24	N Atomic weight	**14**	
	END		

Figure 2-4. A portion of a typical calculation worksheet for a process unit (precipitation/ultrafiltration unit)

The composition of some of the feed streams also can be linked directly to the composition of the envelope streams. In that case, the user only needs to specify the percentage each of the envelope streams contributes to the feed stream and the total volumetric flow rate. The model calculates the composition of the feed stream automatically if it is linked to the envelope streams.

2.2.5 Process Dependent Input Streams

Process dependent input streams are those streams directly associated with the process units. Their properties change with the process parameters of the individual process units. For instance, the precipitation agent stream in the precipitation/ultrafiltration unit depends on the pH and strontium concentration in the main input stream (Stream 20), the solid percentage in the output stream (Stream 24), and the filtration efficiency of the filtration unit. The properties of the process dependent streams can be calculated given the process parameters of the process unit and the properties of the streams associated with the process units. Because the data in these streams do not need to be specified by the user, they only appear in the process unit worksheet.

2.2.6 Summary Tables

Two worksheets are provided that summarize the properties of all streams in the pretreatment flowsheet. One of these worksheets summarizes the mass-balance properties and the other summarizes the radioactivity balance properties.

2.2.7 Font Style Rules

In the spreadsheet, if the cell contents are either in **bold** or *italic* font style, the value in the cell is derived from other cells using a formula [i.e., the value is dependent on other value(s) and it cannot be changed manually]. The PRETREAT user interface is designed to not allow modifications to the values or texts in those cells whose contents are in **bold** or *italic* (see section 3.3).

3 USER INTERFACE

Because the pretreatment flowsheet is a complex system and involves a large number of processing data, more than 20 worksheets are used in PRETREAT. It will be difficult for a user to manually navigate through the various worksheets to correct or make changes to specific values or equations. Therefore, a user interface is implemented to

(i) Guide the user in navigating through the worksheets and finding locations of cells (variables) that require modification.

(ii) Minimize the tendency of the user to make incomplete specifications directly on the worksheet. For instance, the user interface has built-in commands that prompt a user to verify an entry before a change is applied.

(iii) Enforce other useful rules, such as those that prevent a user from accidentally entering data in cells that contain mathematical formulas or from making a data entry in a cell that has the wrong data type.

The user interface in PRETREAT is implemented in a Microsoft Visual Basic environment. It consists of forms and control boxes, buttons, and dialogs located on the forms. In the current version (Version 0) of PRETREAT, the user interface has the following forms:

- Main
- Process Units
- Process Parameters
- Process Components
- Solid Assay
- Input Streams
- Streams

These forms and their functions are described in sections 3.1 through 3.6.

3.1 MAIN FORM

The Main form (figure 3-1) is like a switch board in an organization office. On opening the spreadsheet file, the Main form automatically appears and the user can make appropriate selections from the Main form to perform certain tasks. When the Main form is active, the worksheet that contains the flowsheet (figure 2-1) will be displayed in the background underneath the Main form.

The Main form presents the user with two groups of functions to select. One function group is related to working with the worksheet. The buttons for this function group are inside a frame box, marked Spreadsheet/Flowsheet. The other function group is related to working with the user interface.

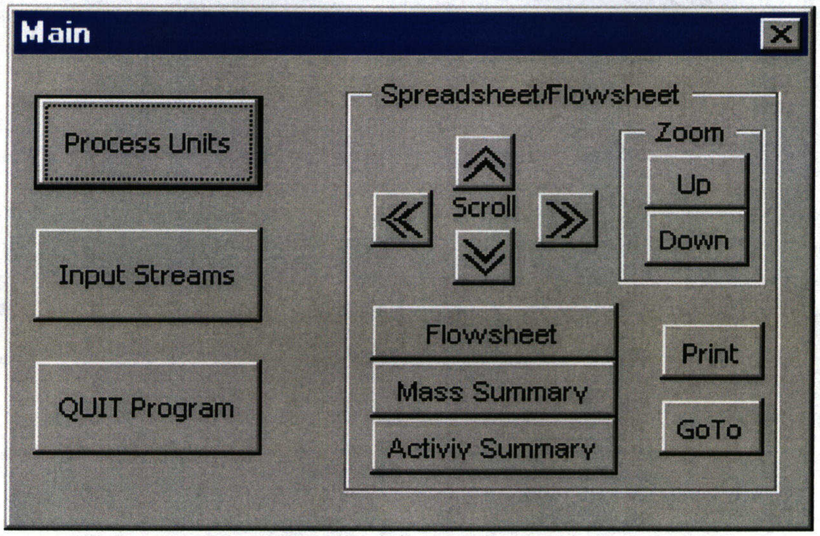


Figure 3-1. The Main form of the PRETREAT user interface

3.1.1 Functions Related to the Spreadsheet/Flowsheet

<u>Scroll Buttons</u>

The Scroll buttons allow the user to shift the worksheet underneath the Main form up, down, left, or right, as indicated by the arrows, to have a better view of certain portions of the worksheet. To see the worksheet underneath the form, the user can also use the mouse to move the form by holding (pressing the left button of the mouse) the title bar (top portion of the form) and dragging the form.

<u>Zoom</u>

The user can zoom up or down to provide a better view of the worksheet.

<u>GoTo</u>

While the Main form is displayed, the user cannot access the functions in the Excel spreadsheet window. If the user wants to access the Excel functions, such as to print or to simply move the user form out of the way, the user can click on the GoTo button. This closes the Main form and displays the underlying worksheet. To prevent the user from accidentally changing the data in the worksheets, the worksheets are lock protected. If the user wants to make any changes on a worksheet directly, the user must go to the Tools option on the menu bar, select Protection, and choose the Unprotect sheet function. It is recommended, however, the user only make changes through the user interface. Making changes directly on the worksheet may lead to deleting important data or formulas in the worksheet.

In the worksheet, the user can also view the Visual Basic codes by clicking Tools on the menu bar, choosing Macro, then selecting Visual Basic Editor. Visual Basic Editor will be launched and the codes can be viewed by choosing View in the pull-down menu, then clicking on Code.

As mentioned in section 2.2.2, there are two command (Visual Basic) buttons—To Main Form and To Previous Form—on every worksheet in PRETREAT. The To Main Form button takes the user to the Main form (no matter which worksheet the user is currently on) and the To Previous Form button takes the user to the last form the user worked with.

Print

The Print button allows the user to print the worksheet underlying the Main form. The print setup or options can be changed after the Print button is clicked. If a user needs to print a certain area of the worksheet, he or she may have to use the GoTo button to close the user form and print directly from the worksheet. After printing, the user can click on the To Previous Form to come back to the user form.

Flowsheet

The Flowsheet button allows the user to place the Flowsheet behind the main user form.

Mass Summary

The Mass Summary Flowsheet button allows the user to place the Mass Summary worksheet behind the main user form.

Activity Summary

The Activity Summary button allows the user to place the Activity Summary worksheet behind the main user form.

3.1.2 Functions Related to Working with the User Interface

Process Units

This button takes the user to the Process Units form, which is a subuser interface (see section 3.2), to modify, view, or print the data or flow diagrams of a process unit.

Input Streams

This button takes the user to the Input Streams form (see section 3.6) to specify, modify, or view the parameters of the independent input streams for all the pretreatment operations.

Quit Program

This button terminates the program and exits PRETREAT. On quitting the program, Excel will ask the user to save the workbook (saving the workbook also saves the embedded Visual Basic codes automatically).

3.2 PROCESS UNITS FORM

Figure 3-2 shows the Process Units form. In this form, the user can select a process unit from a drop-down list box at the top. Once a process unit is selected, the corresponding worksheet will appear automatically (figure 2-3) and the user can manipulate the worksheet. The GoTo button in the Spreadsheet frame is similar to that described in section 3.1.1.

In the Assumptions frame, the user can click on the Process Parameters button to go to the Process Parameters form (see section 3.3). In that form, the user can specify or modify the assumptions or process parameters (the data in the right table of figure 2-4) used in the calculations for the process unit operation.

Inside the Input Stream is Composed of frame, there are three option boxes. If the process selected by the user supports an Auxiliary Input Stream (see figure 2-1), the option buttons related to the Auxiliary Input Stream will be enabled and the user can select the options or choose to modify the Auxiliary Input Stream.

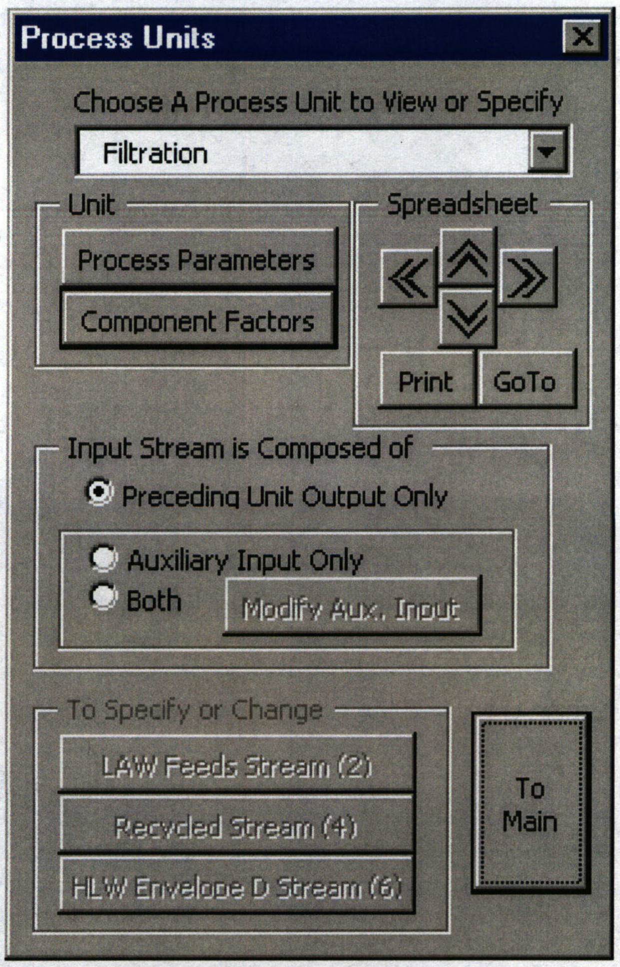


Figure 3-2. Process Units form of the PRETREAT user interface

The To Specify or Change (feed streams) Frame is only enabled when the user has chosen to work on the Feed unit. In this frame, the user can choose to view or modify any of the listed streams. On clicking one of these buttons, the corresponding worksheet for the stream properties (figure 2-2) will be displayed along with the user form, the Streams form (see section 3.7). The user can modify the parameters of the streams through the Streams form.

3.3 PROCESS PARAMETERS FORM

As mentioned in section 3.2, on clicking the Process Parameters button, the Process Parameters form (figure 3-3) will be displayed along with the calculation worksheet (figure 2-4) of the corresponding process unit. In this form, the user can select parameters to modify from the drop-down list box. The new value and reference source can be entered in the appropriate text boxes. The Back button takes the user to the previous form, and the Main button takes the user to the Main form. The Solid Assay button takes the user to the Solid Assay form (see section 3.5).

Similar to the other forms discussed previously, the buttons inside the Spreadsheet frame are for working on the worksheet.

As mentioned in section 2.2.6, cell contents in **bold** or *italic* are calculated from formulas, and the PRETREAT user interface does not allow modifications to these cells.

3.4 PROCESS COMPONENTS FORM

On clicking the Component Factors button on the Process Units form (figure 3-2), the Components form (figure 3-4) will be displayed, along with the calculation worksheet (figure 2-4) for the corresponding process unit.

Other buttons are similar to the Process Parameters form (see section 3.3).

As usual, the PRETREAT user interface does not allow modifications to those cells in **bold** or *italic*.

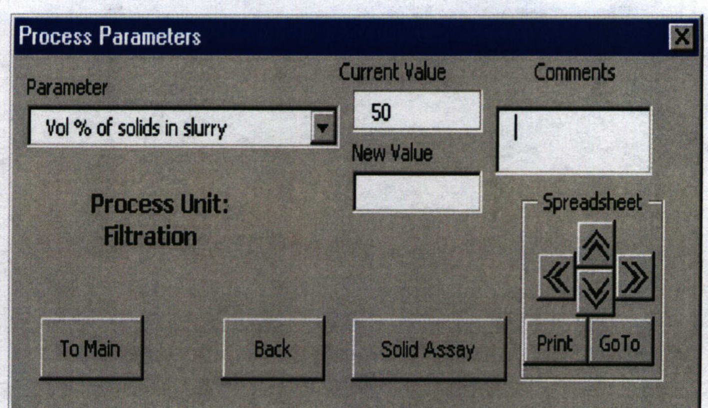


Figure 3-3. Process Parameters form of the PRETREAT user interface

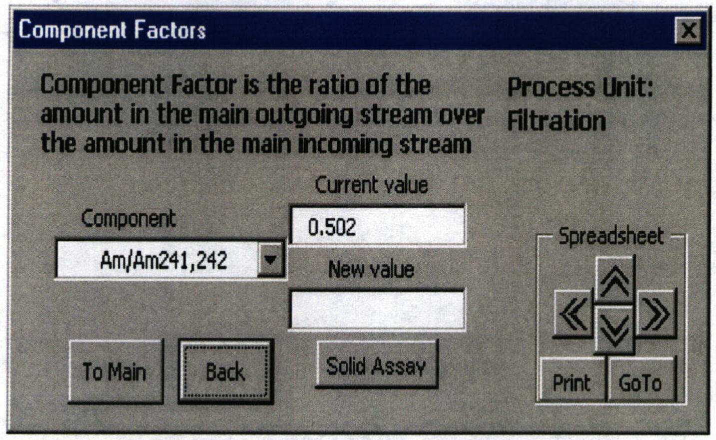


Figure 3-4. Process Components form of the PRETREAT user interface

3.5 SOLID ASSAY FORM

On clicking the Solid Assay button on either the Process Parameter form (figure 3-3) or the Component Factors form (figure 3-4), the Solid Assay form (figure 3-5) will be displayed, along with its corresponding worksheet (similar to figure 2-4). Because the precipitation agent will be added only to the feeds that contain Envelope C waste, there are mainly two types of solids, one for Envelope C feed and the other for non-C Envelope feed. The Solid Assay form allows the user to specify them separately. The model automatically determines which entry to use in the calculation based on the envelope percentage values of the incoming stream.

Other buttons are similar to the Process Parameters form (see section 3.3).

As indicated previously, the PRETREAT user interface does not allow modifications to those cells in **bold** or *italic*.

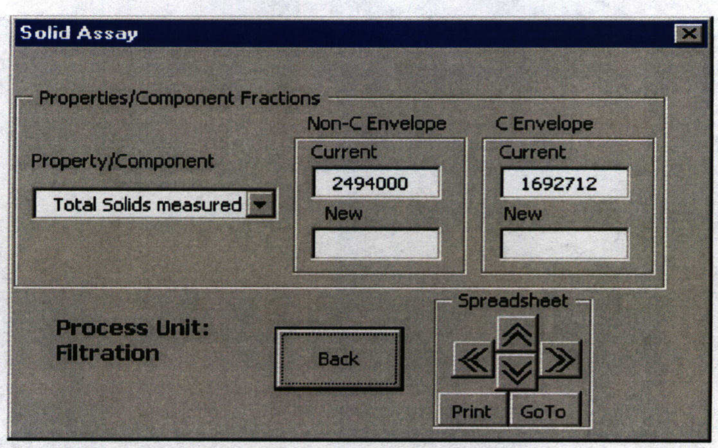


Figure 3-5. Solid Assay form of the PRETREAT user interface

3.6 INPUT STREAMS FORM

As mentioned in section 3.1.2, clicking the Input Streams button displays a user form called Input Streams (figure 3-6). In this Input Streams form, the user can select from the lower drop-down list box an independent stream to modify. Once a stream is selected, the worksheet for the process unit (see figure 2-3) associated with the selected stream is displayed. In the upper drop-down list box, the user can choose to view the flow diagram or view the stream properties of a process unit.

As in the other forms mentioned previously, the buttons in the Spreadsheet frame allow the user to view or work on a worksheet directly.

3.7 STREAMS FORM

Clicking the To Modify button on the Input Streams form (figure 3-6) or the Modify Aux. Input button on the Process Unit form (figure 3-2) displays the Streams form (figure 3-7), along with the worksheet that contains the stream table to be modified. There are mainly two frames, the Stream Properties frame and the Component Properties frame. The Stream Properties frame allows the user to modify stream properties, such as stream name, flow rate, and flow density, and the latter allows the user to specify or change the concentration or activity of the components.

The Back button in the Streams form takes the user to the Input Streams form (figure 3-6) or the Process Unit form (figure 3-2) which ever initiated the Streams form.

The user is referred to section 3.3 for descriptions of the other buttons in the Streams form.

Similar to the Process Parameters and Process Components forms, the user interface does not allow modifications to the cells whose contents are in **bold** or *italic*.

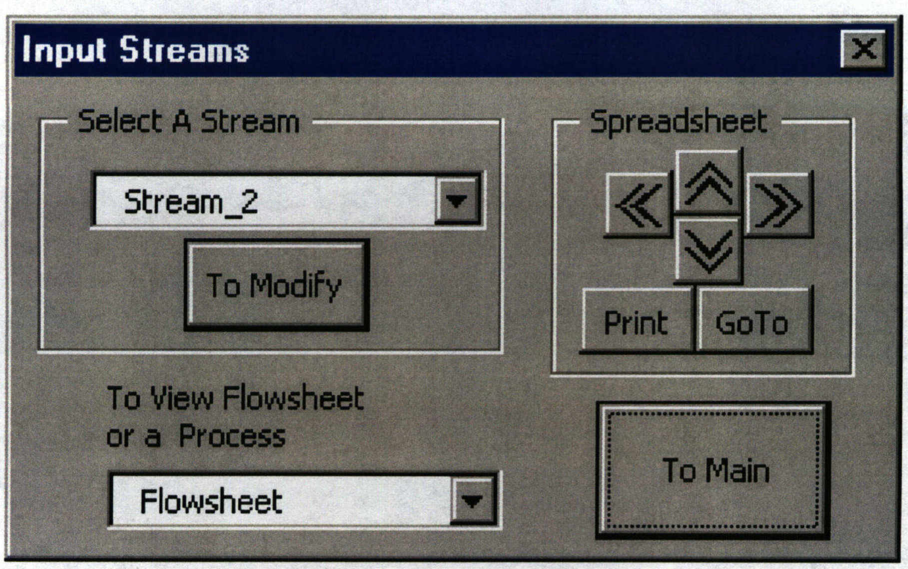


Figure 3-6. Input Streams form of the PRETREAT user interface

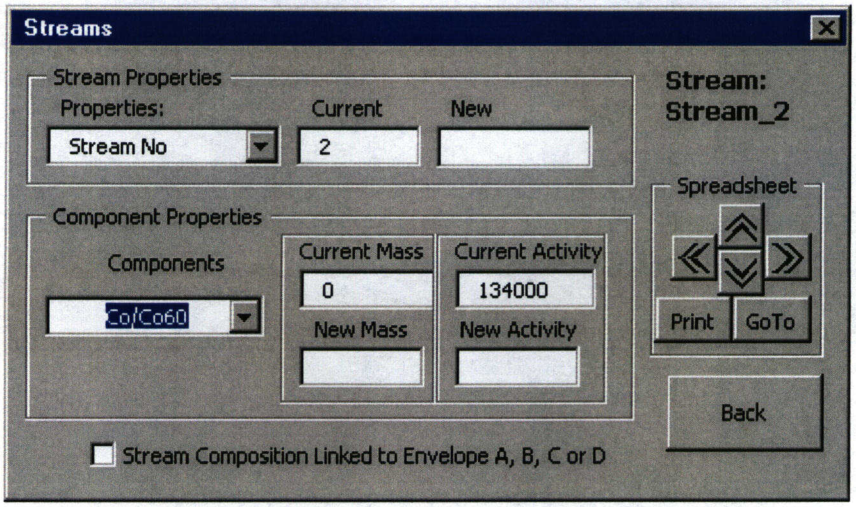


Figure 3-7. Streams form of the PRETREAT user interface

4 HARDWARE AND SOFTWARE REQUIREMENTS

PRETREAT requires Microsoft Excel 97 or a later version running on a personal computer with a Windows operating system (Windows 95, 98, or NT). The user interface is implemented using Visual Basic for Applications that is included in a standard Excel 97 package.

5 RUNNING THE PROGRAM

The file name for the program is Pretreat.xls. The program can be started by opening the file in Excel 97 or a later version, or by double clicking the file name in Windows 95, 98, or NT. Because the file contains Macros, a virus-warning message may appear at the start. Please press the Enable Macros button to continue. This warning is a standard feature of Excel to warn Internet users against downloading spreadsheet files that may contain a virus. The user interface will be displayed automatically.

The original Pretreat.xls file provided with this report is a read-only file. The user will be prompted to save the workbook under a new filename.

6 REFERENCES

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