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Global Modeling of Hanford Tank Waste Pretreatment Alternatives Within a Total Cleanup System Using ASPEN PLUS™

Prepared for the U.S. Department of Energy
Office of Environmental Restoration and
Waste Management

Westinghouse
Hanford Company Richland, Washington

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Introduction

The purpose of this work is to evaluate and compare radionuclide separations/processing technologies being developed or considered as Hanford tank waste pretreatment alternatives. These technologies are integrated into a total cleanup system that includes tank waste retrieval, treatment, and disposal. Current Hanford flowsheets typically include only mature, developed technologies, not new technologies. Thus, this work examines the impact/benefits of inserting new technologies into Hanford flowsheets.

Waste treatment must produce disposal fractions which are less troublesome than the original material. Researchers seeking effective treatment methods may lack the tools or expertise to fully understand the implications of their approach in terms of secondary and tertiary waste streams or the extent to which a unique new process will affect upstream or downstream processes. This work has developed and demonstrated mass balance methods that clarify the effect of including individual processes in an integrated waste treatment system, such as the Hanford cleanup system. The methods provide a measure of treatment effectiveness and a format for the researcher to understand waste stream interrelationships and determine how a particular treatment technology can best be used in a cleanup system.

Following is a description of the Hanford tank waste cleanup model developed using the ASPEN PLUS[1] flowsheet simulation tool. Important aspects of the modeling approach are discussed along with a description of how performance measures were developed and integrated within the simulation to evaluate and compare various Hanford tank waste pretreatment alternatives.

Hanford Tank Waste Pretreatment Flowsheets

Numerous pretreatment flowsheets have been proposed for processing the radioactive wastes in Hanford's 177 underground storage tanks. On one extreme are minimal treatment flowsheets containing a few separations which moderately concentrate radionuclides into a High Level Waste (HLW) glass product. To the other extreme are complex flowsheets with dozens of separation processes intended to minimize the HLW volume and radiotoxicity of the Low Level Waste (LLW) glass or grout product. These alternative flowsheets are compared using a mass balance approach to demonstrate the impact of balancing greater capital equipment/operating resources needed for aggressive separations against the reduced waste disposal resources and decreased environmental/health risks. The

[1]ASPEN PLUS is a trademark of Aspen Technology, Inc.

ASPEN PLUS flowsheet simulator is used to perform the mass balance calculations.

The contents of the waste tanks are known only approximately. The assumed composition of the waste stream to be treated can affect conclusions drawn about the relative worth of different pretreatment options. Tank waste streams are defined as though all waste (sludge, supernatant, and salt cake) from all tanks (single- and double-shell) were blended together and processed in a single campaign. This assumption allows the effects of pretreatment options and the various included technologies to be evaluated without forcing discussions about the large number of permutations among retrieval and blending options. Also, it is consistent with assuming that pretreatment will be done in a single, central processing facility. Alternatively, in-tank processing is currently considered as the baseline processing strategy while tank waste blending and retrieval sequencing are now being considered.

Future work will include a sensitivity study in which more than one type of tank waste is specified as input, instead of a single homogenized blend, and where variables describing sludge behavior (i.e., distribution between solid and liquid in feed stream, and fraction dissolved of several components in dissolution steps) are varied to determine the impact on flowsheet performance. Results from this work will identify high-impact areas of uncertainty in sludge processing on which research and development (R&D) should be focused.

Control Of Modeling Complexity

The ASPEN PLUS global model development began with the process flowsheets modeled using the Integrated Computer-Aided Manufacturing (ICAM) Definition (Language) (IDEF) software tool at a higher abstraction or less detailed level showing all major feed and product streams and the main process blocks. The IDEF tool allowed showing the flowsheet description at increasingly decomposed states (i.e., a hierarchical representation) as shown in Figure 1. The higher level model allowed good understanding of the overall waste flow in each process and facilitated the development of a more detailed process model. Each main process and stream in the higher level model was further broken down or decomposed to an appropriate detail level for implementation using ASPEN PLUS. Thus, the IDEF representations became the ASPEN PLUS flowsheet specifications. The global model flowsheet representation for an extensive processing strategy is shown in Figure 2.

This systems engineering or top-down approach for flowsheet model specification enabled lumping (i.e., grouping together of streams, processes, etc.) decisions to be made to control model complexity and tradeoff representation details against modeling time and flexibility. It also increased the ability to do parametrics and sensitivity studies.

The IDEF model flowsheet specifications were used to build the ASPEN PLUS flowsheet model connectivity with all the specified feed and product streams. In place of rigorous chemical and physical process models, the ASPEN PLUS models used simpler mixer, splitter, separator, and reactor models. The mixer blocks combine material streams into one stream. The splitter blocks combine material streams and divide the resulting stream into two or more streams, with all outlets having the same composition and properties. The separator blocks combine streams and separate the resulting stream into two or more streams according to splits or separation factors specified for each component. The reactor blocks simulate chemical reactions by using stoichiometric reaction equations with extents or by simply including specified reaction yields of each component.

The detailed level flowsheet models typically had several hundred blocks, several hundred streams, and up to approximately 170 components or chemical species. This level of detail was necessary to model the unit operations in a complete pretreatment plant layout to facilitate equipment sizing and costing, to accurately account for feedstream changes and the impacts on chemical additions, and to represent the complex tank waste speciation.

To reduce the modeling complexity, global (or intermediate) level models were developed to represent the detailed flowsheet models. These global models were generally about a fifth of the size of the detailed models in terms of the number of blocks, streams, and components, and were self-contained in modeling the tank waste retrieval, treatment, and disposal processes. Process performance measure calculations were implemented within the global models because of their less complex modeling environment.

Rollup Of Detailed Model Results Into The Global Model

To provide accurate process representation in the global model, calculations of stream component masses, stream separation factors, and reactor yield factors were based on the detailed model data. These calculations were automated using spreadsheet scripts (i.e., programs). This automation allows using a variety of block, stream, and component lumping or grouping schemes in processing the detailed model results for implementation in the global model.

The separation factors were based on rolling up (or lumping) the detailed model stream and component data for individual output streams and comparing the component distributions between streams to the total output stream. The reactor yield factors were based on comparing the distribution of component masses in the total output stream compared to the total input stream for a particular process block.

Accurate representation of the detailed model process blocks was achieved in the global model by representing a group of blocks with a reactor and a separator block together. The reactor blocks accounted for component mass changes resulting from chemical reactions within the group of detailed model process blocks while the separator blocks separated those components into their appropriate output streams.

Model Data From Spreadsheets Into The Flowsheet Simulator

Model data (e.g., separation factors, reactor yield factors, feed and chemical makeup stream inventories) were stored in spreadsheet files. These files were changed and maintained separately from the ASPEN PLUS input files. The file data were correlated to the ASPEN PLUS models by their respective block and stream names. These data were processed for inclusion into the ASPEN PLUS input files by spreadsheet scripts. These scripts produced the necessary formatted data statements that could be inserted directly into the ASPEN PLUS input files. Thus, data changes were done quickly and easily within the spreadsheet files and then the scripts placed the data into the proper form for use in the model file.

FORTRAN subroutines were included in the detailed model to output desired stream data into spreadsheet compatible files for processing by spreadsheet scripts. The format of these files was similar to that created by the Model Manager[2] program using the spreadsheet file creation feature. The spreadsheet scripts performed the rollup or lumping of data necessary to represent groups of blocks, streams, and components within a smaller number of respective units.

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[2]Model Manager is a trademark of Aspen Technology, Inc.

This automation generated the majority of data required by the global models directly from the detailed model data. Subsequent processing of the global model output data was again performed using spreadsheet scripts operating on spreadsheet data files generated by the Model Manager program.

These separate data files maintained the block and stream data together in a summarized tabular form for easy review. These summary tables were valuable in tracking component separation factors through several process blocks to more readily understand component flows and eliminate errors. Data modifications were done quickly and easily within the spreadsheet environment. After finalizing the input data the spreadsheet scripts quickly processed the data and produced the new input specifications required by ASPEN PLUS.

Contributions Of The Flowsheet Simulator

The ASPEN PLUS flowsheet simulator provides a tool for rapid development and changes to the Hanford cleanup system model. It provides flexibility to model different unit operations and chemical species, along with feedstream changes. It also automates integration of unit operations along with recycle streams, chemical makeup streams, reactor model specifications representing stoichiometric reactions, and separation specifications representing unit operation performance. It is also flexible in using user-specified FORTRAN subroutines in calculations of stream or process design dependent constraints (e.g., process design constraints were modeled using the design specification feature coupled with user developed FORTRAN subroutines).

The simulation tool supports system analysis and evaluation. The model can be used to study economic considerations such as quantifying the trade-off of greater capital equipment/operating costs for aggressive separations with the reduced waste disposal costs and decreased environmental/health risks. Sensitivity calculations can be performed to quantify the effects of variations in design constraints, feedstream compositions, etc. For example, the effect on the volume of HLW glass product and radiotoxicity of the LLW glass or grout product was predicted for different flowsheet processing alternatives using current assumptions about waste characteristics and separations processes.

The nonlinear optimization features of ASPEN PLUS were used to determine optimal glass waste loadings that met glass property constraints for the vitrified waste products. Significant reductions in the waste glass production were observed when specific limiting constraints were relaxed in the glass optimization calculations. These optimization results have tended to focus more work on finding acceptable glass compositions that will accommodate higher loadings of specific species (e.g., P_2O_5) and allow relaxing some of the binding constraints.

The Model Manager tool provided a rapid method of developing the flowsheet connectivity and generating the associated specification along with a process flowsheet diagram or layout print file. Spreadsheet scripts were written to create connectivity files directly from ASPEN PLUS input data files that could then be imported directly into Model Manager to allow layout of the flowsheet diagram using the place block feature. This was useful in generating flowsheet diagrams for input files created outside of Model Manager and did not require ASPEN PLUS execution. Model Manager was also used to generate spreadsheet files from the ASPEN PLUS output summary files.

Development/Integration Of Process Strategy Performance Measures

Performance measures were developed to allow evaluation and comparison of different process flowsheet strategies. The calculation of these measures were automated using FORTRAN subroutines linked directly in the ASPEN PLUS input specification file. Nonlinear optimization routines provided with ASPEN PLUS were also used. The following describes the performance measures used in the Hanford tank waste cleanup system model and their integration in the simulation model.

Waste Product Generation: Glass Waste Loading Optimization

The currently favored disposal form for both high and low level radioactive waste (HLW and LLW, respectively) is a borosilicate glass. The waste will be combined with glass formers whose composition is selected based on the composition of the waste to be vitrified. In this context it is assumed that large volumes of waste of nearly constant composition will be processed in a series of campaigns. An appropriate glass former composition will be selected to maximize the waste loading in the resulting glass; substantially different waste loadings can result.

The three general types of constraints on waste loading in the glass are: (1) constraints on the properties of the homogeneous glass when in the melter (e.g., viscosity) or on the properties of the glass after cooling (e.g., durability); (2) constraints on heat loading (or possibly radiation levels); and (3) constraints on the solubility in molten glass of species, such as SO_3, Cr_2O_3, and noble metal oxides that can render the molten glass inhomogeneous, or constraints on the loading of species, such as P_2O_5 that can inhibit the vitrification rate in some melter designs.

A detailed oxidation model was included in the ASPEN PLUS models to accurately account for oxide creation during the waste vitrification process. The resulting oxide product stream was used in a nonlinear glass composition optimization routine to find the maximum waste oxide loading in the glass along with the glass former composition. The optimization accounted for waste glass property constraints (viscosity, electrical conductivity, durability-boron release), heat loading constraints, critical solubility constraints, and single- and multiple-component constraints.

Process Capital And Operating Cost Functions

Cost functions were developed to predict the cost of facilities or activities based on input parameters, such as design throughput capacity, degree of chemical separation, amount of material treated or disposed, or other parameters as needed. Consequently, the cost functions were able to predict costs over a wide range of possible system configurations, rather than for just one specific configuration.

Cost function terms depending on design throughput capacity were based on the well known exponent scaling method where the ratio of the desired capacity to a reference capacity is raised to an exponent between 0.0 and 1.0 as shown below.

$$(\text{Actual capacity / Reference capacity})^{\text{Exponent}}$$

One of these terms is multiplied times a reference capital cost to obtain a capacity-scaled capital cost. A similar term (generally with a different exponent) is multiplied times a reference operating cost to obtain a capacity-scaled operating cost. Many published tables of suggested exponents exist for specific chemical processes and processing facilities. Where no process-specific exponent could be found, a generic value of 0.7 was often used for the capital cost component. A value of 0.75 is usually used for the operating cost component.

Cost function terms, depending on the degree of chemical separation, were based on the estimation that precipitation processes tend to have costs that increase linearly with increasing separation, solvent extraction processes tend to have costs that increase as the logarithm of separation, and ion exchange processes tend to have costs that increase as the logarithm of separation raised to the 0.55 power. These functional dependencies were semiquantitative estimates based on first principles considerations.

Typically, individual cost functions were developed by multiplying together terms that correct for throughput capacity and terms that account for desired separation (if applicable). In instances where no separation is involved, an appropriate cost term was often simply multiplied times the total volume of waste involved in the process or facility. In other, unusual cases, some other scheme for developing the final cost function was used, but in all cases, the end result was some combination of curve fitting, exponent scaling, and assumed functional forms for the process or activity under consideration.

Tertiary Waste Generation

Whenever separation processes are added to any given separations scheme, further addition of process chemicals and associated generation of waste will occur. The term "secondary waste" is often used to describe waste resulting directly from the routing of process chemicals to an effluent stream, to distinguish it from "primary waste," which is the waste retrieved from HLW tanks. Secondary waste can be minimized by recycle and careful selection and integration of the separation processes. The predicted generation of secondary waste was computed as part of the mass balance model approach.

The term "tertiary waste" was used to describe various nonprocess waste streams or wastes that did not result directly from splitting or partitioning of the main process streams. This waste includes trash and incidental capture of liquid and solid emissions. For example, included as noncombustible materials (e.g., glass, metal, and soil) are items such as contaminated or irradiated equipment, waste and spill site soil, silver-coated packing material, smoke detectors, and basin sediment sources (e.g., ^{57}Co, ^{137}Cs, ^{239}Pu, ^{235}U). Included as combustible materials (e.g., absorbents, cellulose, plastic, rubber, liquids) are items such as toxic cleanup material, laboratory waste, filter cartridges, deionizer resins, contaminated clothing, lubricants, solvent waste. Included as aqueous wastes are items such as scintillation solution, high- and low-activity waste, and decontamination solutions. Because data for cell air and offgas rates were not available, the volume of filters (e.g., high-efficiency particulate air filters and in-tank precipitation filters) resulting from offgas treatment was substituted.

The generation of tertiary waste was estimated and included in the mass balances. However, these estimates were necessarily rough, being based on the generation of similar wastes during operation of large chemical plants at Savannah River, Hanford, and other Department of Energy (DOE) sites. The estimates are probably conservative relative to operation of future facilities, assuming waste minimization will be a design and operating objective. The mass balances also include estimates of the chemical adds for tertiary waste treatment.

Health Hazard Indexes (Short And Long Term, Occupational)

Systems analyses of radioactive waste handling systems require safety performance measures in evaluating alternative processes. Absolute health risks in terms of dose or deaths are not necessary for the purpose of process comparison. Only ratios of health risks of the same kind were calculated for the processes to be compared. Health risks of each kind were stated as ratios to a standard or a regulation, and the values for each process were compared with each other.

The various kinds of health risks can be subdivided into short term and long term with the time of decay of ^{137}Cs and ^{90}Sr to insignificant values as the transition point. In waste repository risk calculations, the range 300 to 1,000 years after reactor discharge was used as a transition range. Therefore, a transition range of 500 years was used as the dividing time between short term and long term in the systems studies.

A second kind of subdivision of health risks is between onsite and offsite risks. The term "onsite risks" refers to radionuclides or chemicals in question that remain onsite usually in solid form and undisturbed unless man intrudes and releases them into the biosphere, exposing himself or carrying them offsite to expose others. The term "offsite risks" refers to radionuclides or chemicals that migrate offsite with geochemical agents, such as water after barriers are breached. The onsite risk is directly related to the concentration in the waste at the onsite sample point, while offsite risk also depends on the solubility in water and the rate of transport to a remote sample point where the material is released to the biosphere.

A preliminary division of the safety performance measures into five categories was made, and a relative health risk estimate for each of them was developed. The categories are given below:

1. Long-Term Offsite Safety: This measure was confined to radionuclides that can be transported by water from the waste site and measured by an adjusted health hazard index (HHI). The important nuclides within the time scale of a HLW repository are ^{99}Tc and ^{129}I.

2. Long-Term Onsite Safety: This measure assumed that human or animal intrusion will introduce mixed wastes directly into the biosphere. This measure was represented by the ratio of radionuclide concentration to Hanford cleanup residential soil standards. The important nuclides are alpha emitters, such as ^{238}U, ^{239}Pu, ^{241}Am, ^{243}Am, and their decay chains.

3. Short-Term Offsite Safety: This measure was confined to radionuclides that can be transported to the biosphere within 300 to 500 years by water or air after unusual events, or which are already present in the groundwater. It is measured by the ratio of concentration to potable water limits. The important radionuclides should be ^{3}H, ^{137}Cs, and ^{90}Sr.

4. Short-Term Onsite Safety: This measure assumed human or animal intrusion will introduce mixed wastes directly into the biosphere within 300 to 500 years. This measure was represented by the ratio of radionuclide concentration to Hanford Site cleanup residential soil standards. The important nuclides should be ^{137}Cs, ^{90}Sr, and ^{239}Pu.

5. Occupational Exposure: This measure accounts for exposure to workers operating the processing plants who are taking samples and cleaning up spills. It is directly proportional to and measured by the volume and activity level of tertiary nonprocess wastes, such as special work permit clothing, laboratory

samples, gloves, removed equipment, and decontamination solutions. The important radionuclides should be ^{137}Cs, ^{90}Sr, and ^{239}Pu. These may be classified as gamma fields, alpha emitters, and beta emitters with low energy gamma fields, and indexes can be calculated separately for each category.

It is certainly desirable to evaluate all five of these relative performance measures separately. However, after this step is taken, one cannot combine them into a single safety performance measure without calculating the risk from each (i.e., the product of probability of occurrence and the dose consequences). The following describe how each of these health measures was evaluated.

Long-Term Offsite Health Hazard

The long-term offsite radiological safety performance measure was evaluated by combining transport through a barrier to a 100 meter distant well with the concentration limit for potable water. The resultant adjusted HHI was then used to compare the waste separation alternatives. This long-term performance measure is confined to radionuclides that can be transported by water from the waste site and measured by the adjusted HHI. Again, the important nuclides are ^{99}Tc and ^{129}I.

Long-Term Onsite Health Hazard

A preliminary set of coefficients for long-term onsite health hazard was developed for the global model lumped components. These coefficients were derived from the drilling and excavation scenarios previously studied in dose and risk assessments for intrusion into mixed waste disposal sites. For all situations, the dose from the excavation scenario predominated over the drilling scenario. The study results were presented in terms of rems per person per drilling or excavation event for individual radionuclides present at unit concentrations in the solid waste. They represented the worst-case scenario with pathways to the highest exposed individual.

To calculate the long-term onsite HHI (mrem per person) associated with a particular component in a specific waste stream, the HHI coefficient (mrem/[Ci/m3]) for that component was multiplied by the radioactivity level (or concentration) (Ci/m3) of the component in that specific waste stream.

Short-Term Onsite And Offsite Health Hazard

The offsite health hazard for the short term (less than 500 years) was nearly nil because the barriers to migration would be expected to be intact and unbreached for 500 years unless man intruded. Therefore, the offsite health hazard was included in the onsite health hazard. The short-term onsite health hazard was calculated in the same way as the long-term onsite health hazard, except that the age of the waste was assumed to be only 10 years so that ^{137}Cs and ^{90}Sr were still the dominant radiation dose inventories.

Occupational Exposure

The dose to workers operating a plant may be an important health hazard. In general, with similar designs, one would expect that more highly radioactive streams result in greater worker exposure, even though the processes themselves are shielded. This is because sampling and equipment repair usually have some doses associated with them. It was arbitrarily assumed that the occupational exposure was proportional to the volume of tertiary nonprocess waste from a particular process multiplied by the curie concentration of the lumped component in the feedstream to a process. This does NOT result in the curies in the tertiary waste or in an HHI in terms of dose but does leave the possibility that the index could be calibrated by data from an operating plant.

There are essentially two types of occupational exposure. They are as follows.

1. Gamma radiation (primarily ^{137}Cs) emanating from equipment, processes, or contamination, which acts through a distance and perhaps requires shielding.

2. Contamination by alpha and beta particles where the radionuclide gets on the clothing, skin, or inside the person. The alpha contamination is quite significant in occupational exposure (e.g., uranium, plutonium, neptunium, thorium, americium). The beta contamination will be unimportant unless a low-energy gamma accompanies the beta decay.

Thus, the occupational exposure HHI was calculated for each major process using three separate indexes for gamma, alpha, and beta contamination. These indexes represent the process feedstream radioactive inventory concentration (Ci/kg) weighted to represent tertiary waste "curies" by multiplying by the process tertiary waste stream inventory (kg). Assuming an arbitrary 1 kg/m3 density for comparison purposes, the resulting HHIs are in units of curies times kilograms per cubic meter. Note that by calculating the HHIs for each process, due credit is given to flowsheets in which high-dose radionuclides are taken out of streams in the earlier processes, leaving lower potential for exposure in downstream processes.

Waste Classification And Radionuclide Concentrations

The radioactivity level (or concentration) of each component in each waste stream was determined by making a global level model run using the radioactive curie inventories in place of the kg mass inventories for the tank waste feedstreams. Multiplying the component curies (Ci) in a specific waste stream by the waste stream density (kg/m3) and dividing by the total waste stream kg yields the desired component radioactivity levels (Ci/m3).

Process Strategy Technical Risk

The development of a process strategy technical risk estimation method was based on data showing various alternative process technology development levels and extents. This data was tabulated using the following categories:

- Maturity of particular process technologies - extent and scale of testing with simple or realistic simulants (e.g., laboratory, bench, pilot plant, full scale, operating full scale facility);

- Potential benefit of particular process technologies - activity level and timeliness of testing and development; and

- Current Department of Energy funding level of particular process technologies - extent of funding and the associated advance of maturity.

To allow an assessment of the technical risk associated with each of the process strategies, weighting factors were assigned to the above process technology development levels and extents. These weighting factor assignments were considered first approximations using reasonable engineering judgement. Using these weights, numerical estimates of technical risk factor indexes were calculated for particular process technologies using the formulas,

Technical Risk Index = 1/(Level Weight * Extent Weight) (R&D and DT&E).
Technical Risk Index = 1/(Level Weight) (Proven Levels).

where,

R&D = Research and Development
DT&E = Demonstration Testing and Experimentation.

Summary

A mass balance approach using the ASPEN PLUS flowsheet simulator was developed to clarify the effect of including individual processes in an integrated waste treatment system, such as the Hanford cleanup system. Applying a systems engineering or top-down approach for flowsheet model specification enabled lumping decisions to be made to control model complexity and tradeoff representation details against modeling time and flexibility.

The use of spreadsheet scripts or programs provided a flexible and automated modeling environment to develop and summarize the model data. Maintaining the model specification data in separate spreadsheet files outside of the ASPEN PLUS input files allowed rapid specification data changes, quick tracking of component separation flow, and provided a convenient tabulated set of input specifications. Spreadsheet scripts were developed to process these data to create the required ASPEN PLUS input specification. Included in this automation was the ability to generate Model Manager connectivity files directly from ASPEN PLUS input files that were developed outside of the Model Manager tool.

Several special features of the ASPEN PLUS flowsheet simulation tool were used to provide flexibility in the system models. These features included the use of user-developed FORTRAN subroutines to control design specifications and process conditions for unit operations and their associated chemical additions. Performance measures developed to compare process technologies were integrated directly into the flowsheet model using FORTRAN subroutines. These measures included process capital and operating costs, tertiary nonprocess waste generation, and health hazard index calculation. The nonlinear optimization feature was also used to calculate optimal waste loadings in the waste glass disposal product using constraints based on glass melter properties, heat loading limits, and specie solubility limits.

Figure 1. IDEF STRUCTURED FLOWSHEET

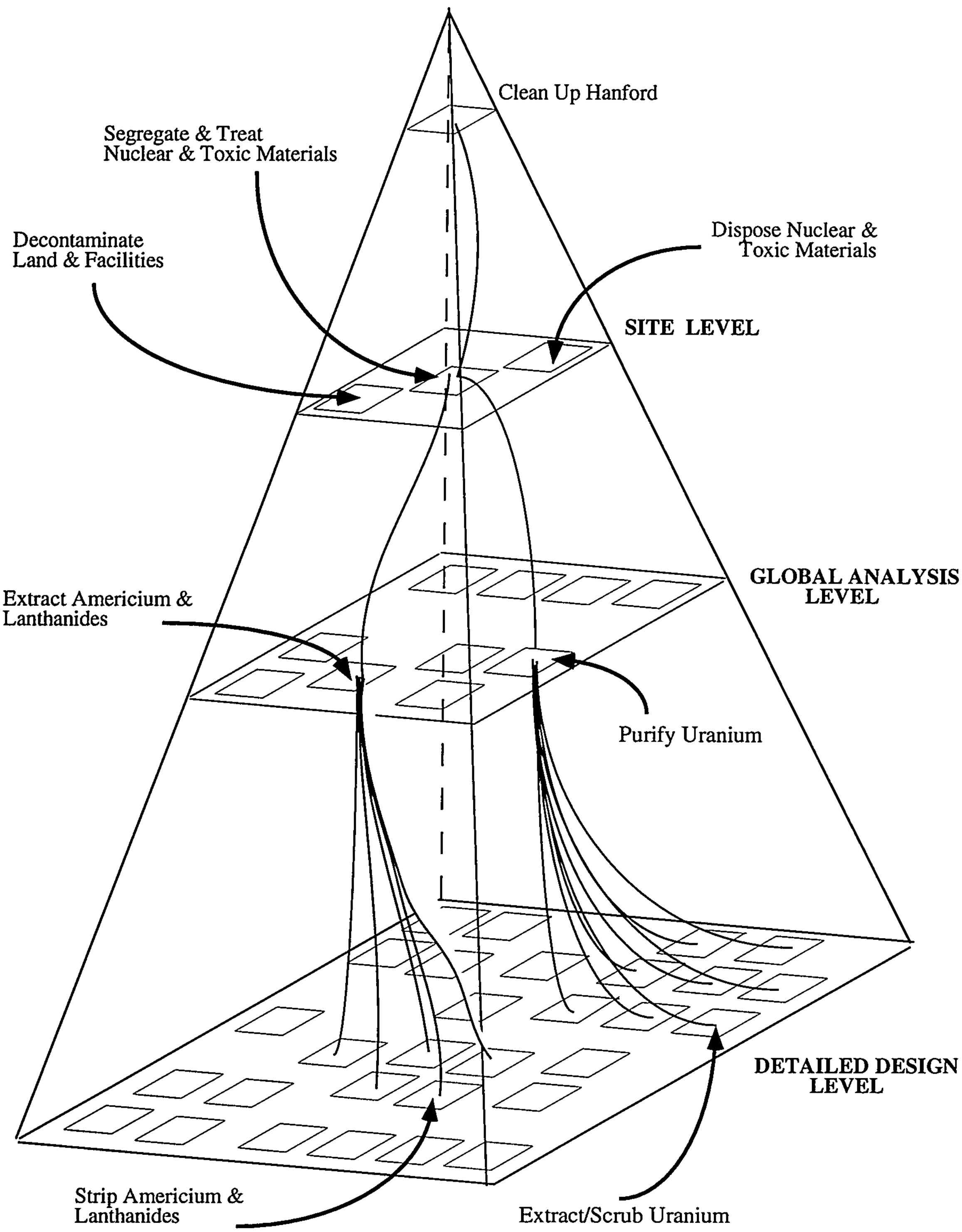
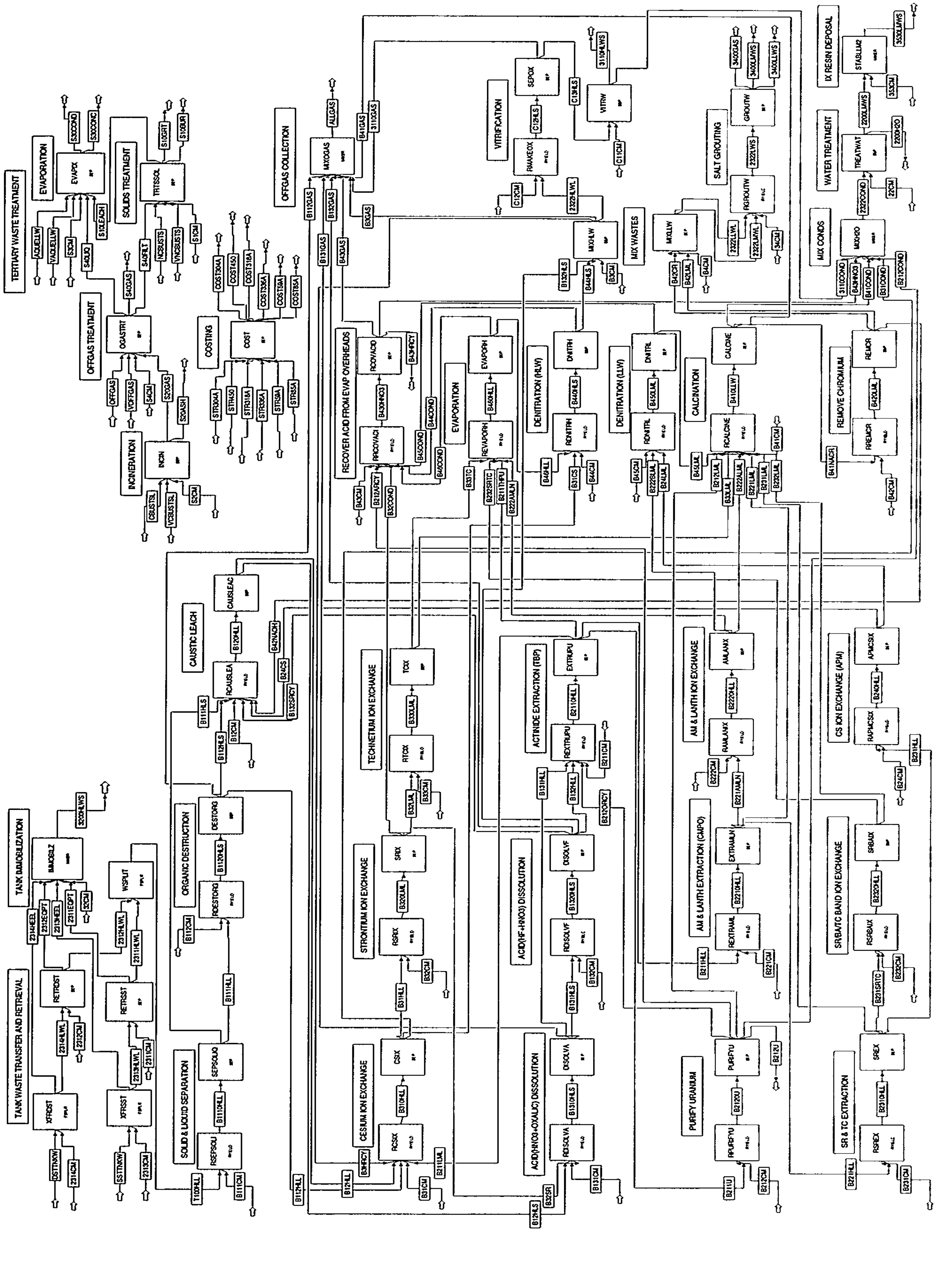


Figure 2. Extensive Separations Global Model



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