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Development of Integrated Process Simulation System Model for Spent Fuel Treatment Facility (SFTF) Design: Quarterly Progress Report January 1-March 31, 2006

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Task 24: Development of Integrated Process Simulation System Model for Spent Fuel Treatment Facility (SFTF) Design

Quarterly Progress Report 01/01/06- 03/31/06

UNLV-TRP University Participation Program

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Research highlights

- The UNLV developed TRPSEMPro software package can access engineering modeling software, ASPEN Plus through its own interface. The new interface eliminates the user interaction with the complex ASPEN Plus package and also provides input and output results for analysis purpose. The current interface will keep improving on collecting multiple scenario runs and database population.
- Two separation processes, acid and plutonium separations, are near completion. The unit operations were finished while some sensitive chemical data for certain species are unknown. Graduate student, Matthew Hodges, continues on finishing those processes using dummy values for those restricted variables. Once the processes complete, researchers from the Argonne National Laboratory (ANL) can plug in the actual values for further evaluation.

Technical progress report

1. Interface to interact with ASPEN Plus through the TRPSEMPro Package

1.1. To generate the interface between TRPSEMPro and ASPEN Plus, two major element types, "Streams" and "Blocks", in ASPEN Plus are identified. Streams can be further divided into two parts, Input and Output that hold the values before and after simulations. Blocks are used to retrieve more system related information.

1.2. The interface shown in Figure 1 provides following functions:
- 1.2.1. The "Browse" button allows the interface to access ASPEN Plus BKP files.
- 1.2.2. The "Process" function interacts with the ASPEN Plus and return simulation results back to the interface.
- 1.2.3. The "Save As" function is the font-end of the database population and multiple run data collector. The function will be executed transparently on the background for compiling report for analysis.

1.3. Since the AMUSE code needs to be part of the optimization process, it will be integrated as a user defined function (UDF) associated with the ASPEN Plus. The optimization strategy between ASPEN Plus and AMUSE simulations need to be formulated soon.

1.4. Chemical flow conventions are different between ASPEN Plus and AMUSE, therefore, conversion process is required.
1.5. The simulation results can be generated iteratively. Database tool will be implemented for data management.

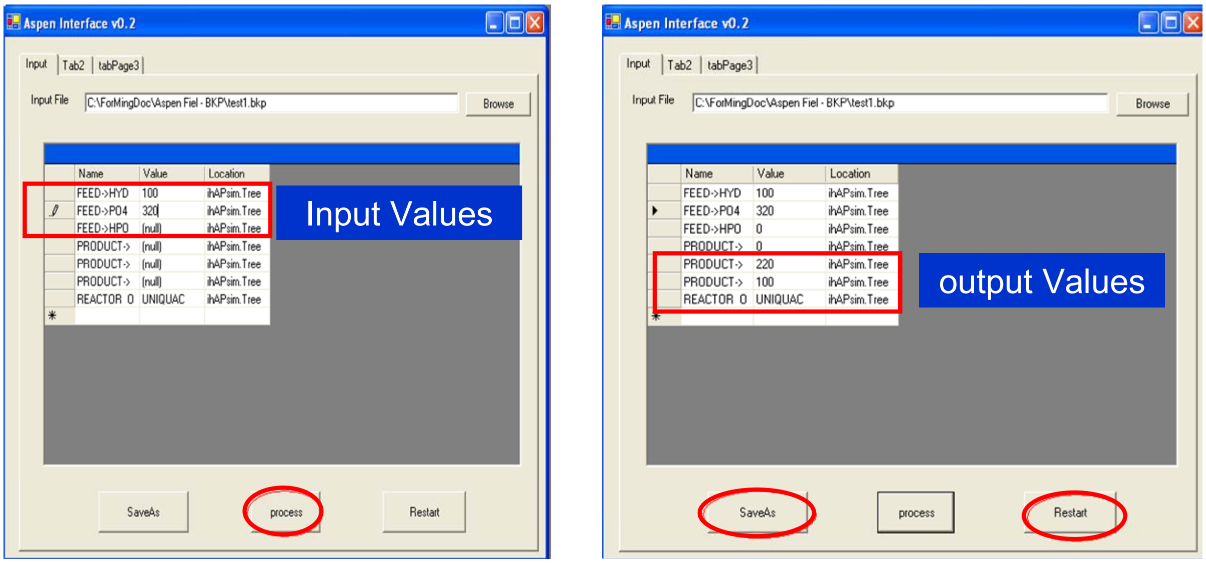

Figure 1. Interface for accessing ASPEN Plus package.

2. Construction of detailed ASPEN Plus separation processes

2.1. There are two processes, acid and plutonium separations, near completion. Unit operations associated with those processes are finished. Chemical data for certain species are still unknown. The third process, vitrification, is still under development.

2.2. Acid separation process
2.2.1. Feeds include acetic acid, nitric acid, water, and nitrate salt.
2.2.2. As shown in Figure 2, the top section includes nitric acid and water while the bottom section includes acetic and nitrate salts.

2.3. Plutonium separation process
2.3.1. The plutonium separation system takes the strip product from the NPEX process as its feed as shown in Figure 3.
2.3.2. Three blocks are used to perform the plutonium separation as shown in Figure 4.
2.3.3. Plutonium nitrate in Block 1 is reacted with oxalic acid to produce plutonium oxalate. The output is entered in the Block 2. Plutonium oxalate in Block 2 is then reacted with air to produce plutonium oxide that enters into Block 3 and reacts with hydrogen fluoride to produce plutonium tetra fluoride.

2.4. Vitrification separation process
2.4.1. Virtually no material on vitrification process in literature was found.

2.4.2. Vitrification processes are very time specific (quick cooling of liquids). Certain user defined functions are needed to take into account the time-dependent issue.

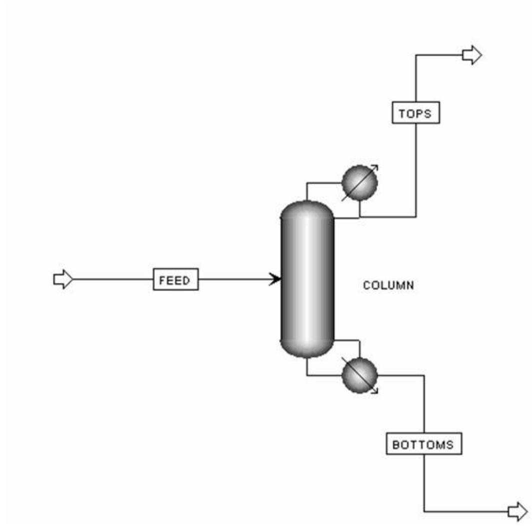

Figure 2. The Acidic separation process.

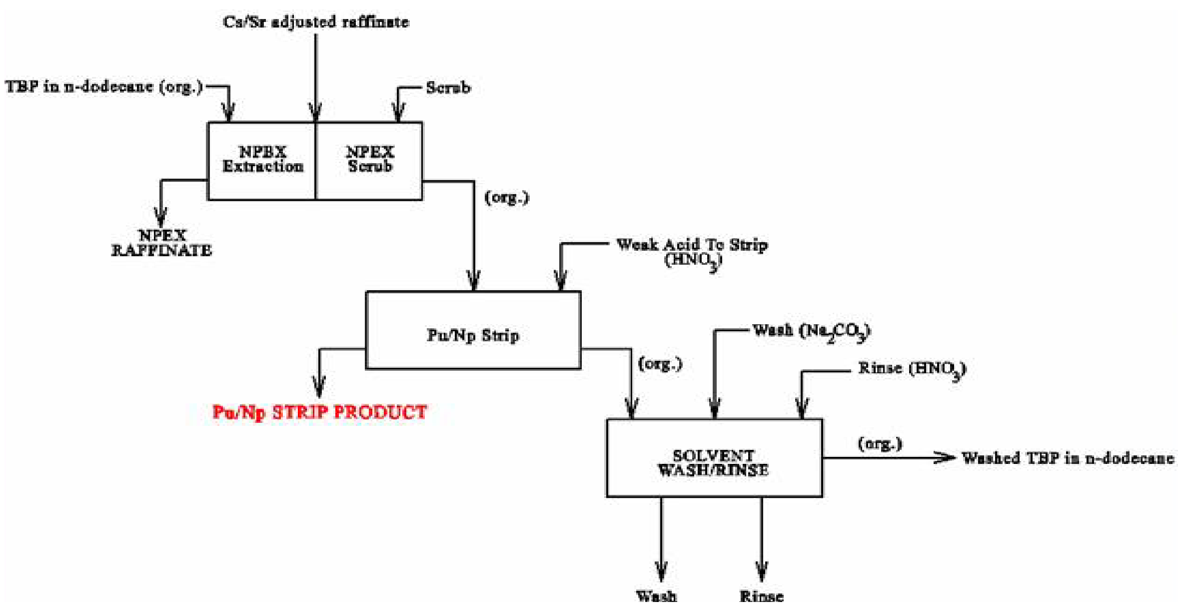

Figure 3. The plutonium separation system that takes the strip product from the NPEX process as its input.

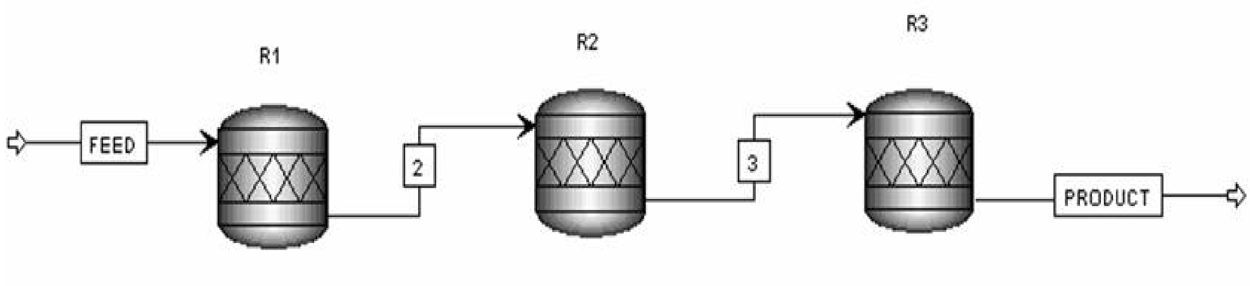

Figure 4. The plutonium separation process.