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Development of Integrated Process Simulation System Model for Spent Fuel Treatment Facility (SFTF) Design: Quarterly Report October 1-December 31, 2004

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

Quarterly Progress Report
10/01/04- 12/31/04

UNLV-AAA University Participation Program

Principle Investigator: Yitung Chen
Co-Principle Investigators: Hsuan-Tsung (Sean) Hsieh

Purpose and Problem Statement

The Advanced Fuel Cycle Initiative (AFCI) and Transmutation Research Program-University Participation Program (TRP-UPP) supported by Department of Energy of the United States have been developing many important technologies for the transmutation of nuclear waste to address long-term disposal issues. While successfully embedding AMUSE module into a dedicated System Engineering Model (TRPSEMPro), developed by the Nevada Center for Advanced Computational Methods (NCACM) at the University of Nevada-Las Vegas collaborating with Argonne National Laboratory (ANL), ANL is interested in further simulating the Light Water Reactor (LWR) Spent Fuel Treatment Facility (SFTF) combining commercial process simulation and analysis packages and core calculation of the AMUSE that derived for using with the UREX+ process. The designed SFTF will receive, temporarily store, and prepare spent nuclear fuel for leaching. The major objectives of this research proposal are to develop a framework for simulating the Spent Fuel Treatment Facility (SFTF) process using AMUSE code, commercial process package such as ASPEN-PLUS, HYSYS and PRO/II and system engineering model such as TRPSEMPro's flexible parameter optimization modules, to develop a middleware package that can communicate between the AMUSE code and any selected commercial packages, to extend the existing system engineering model for optimization process that includes process simulation results, and to include a scenario-based database system that efficiently reports required information as chart output using web-based programming, and Microsoft Visual Basic (MS VB).

Personnel

Principle Investigator:

- Dr. Yitung Chen (Mechanical Engineering)

Co-Principle Investigators:

- Dr. Hsuan-Tsung (Sean) Hsieh (Mechanical Engineering)

Graduate Students:

- Mr. Mathew Hodges, M.S. Graduate Student, (Mechanical Engineering)

National Laboratory Collaborators:

- Dr. George F. Vandergrift, III, Senior Scientist, ANL-East
- Dr. James J. Laidler, Senior Scientist, ANL-East

Management Progress

Budget Issues:

- N/A

Student Issues:

- We need to recruit another graduate student.

Management Problems

No management problem issues at this time.

Technical Progress

1. Kick-off meeting was held in UNLV (10/12-10/14)

    1.1. During the meeting the framework of the system was proposed, discussed and finalized as shown in Figure 1. Major parts of the system are
        - TRPSEMPro (System Engineering Model System Developed by NCACM)
            - AMUSE Simulator- connector between TRPSEMPro and AMUSE
            - ASPEN-PLUS Simulator - connector between TRPSEMPro and ASPEN-PLUS
            - Optimization – analysis module interacts with the above connectors
        - ASPEN-PLUS (commercial process analysis software)
        - AMUSE (Excel macros developed by Argonne National Laboratory)

    1.2. The simulator serves as a middleware that connects between our TRPSEMPro and any external software packages, such as ASPEN-PLUS and AMUSE. A conceptual middleware design for AMUSE Simulator is shown in Figure 2 that includes Single Run, Multiple Run and Optimization functions.

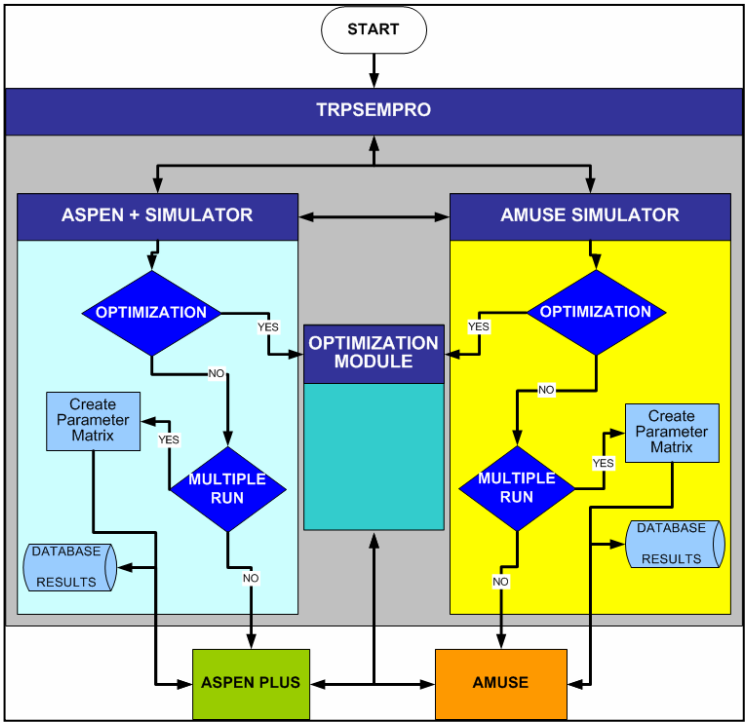

Figure 1 The framework design for the chemical separation process

1.3. Objective functions for the optimization process are needed for implementation of optimization process for the years 2 and 3. Dr. Vandergrift will provide those functions in a timely fashion.

1.4. ASPEN-PLUS is a new process package for the ANL. Currently the NCACM has few academic licenses and will provide some hands-on exercise for the ANL researchers. Meanwhile, the ANL will provide some sample cases and identify process blocks that are related to the chemical separation processing.

1.5. The NCACM team will still consider the ASPEN process as a black box process. The ASPEN Simulator will build around the block and read in the information from the black box and return results to the designated text file or database.

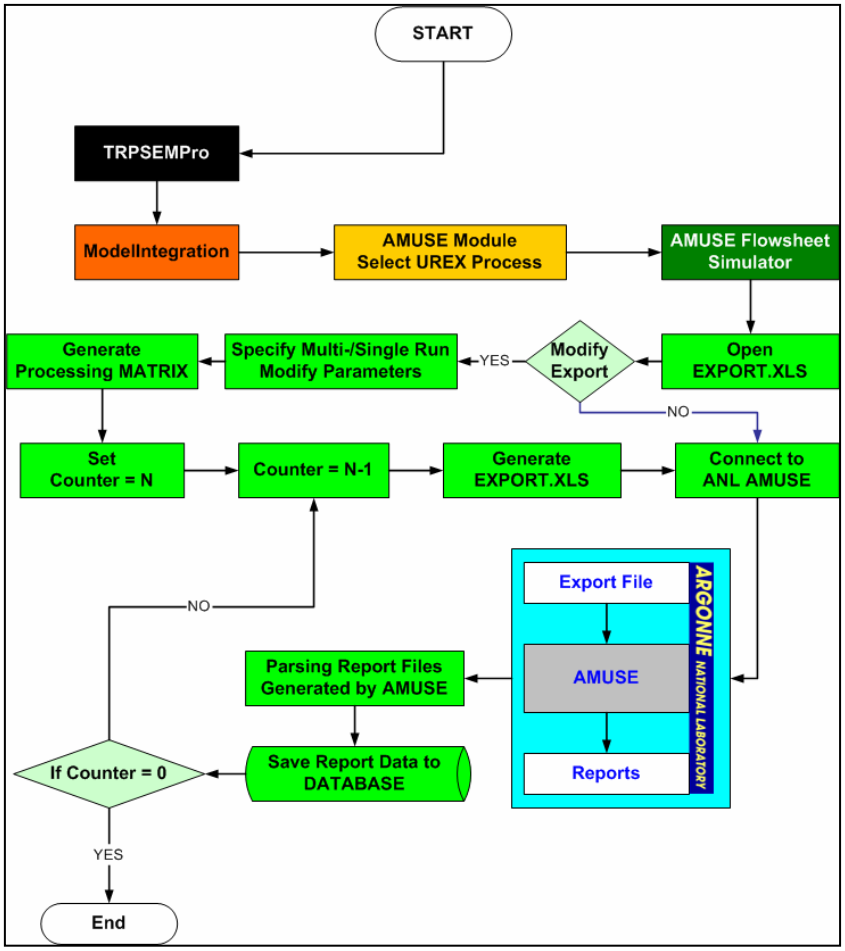

Figure 2 Middleware design flowchart for the AMUSE Simulator.

1.6. The ASPEN-PLUS package exposes its data objects that can be easier to be connected by programming software, such as Visual Basic. The NCACM graduate student has started to familiar with the package, while the ANL will provide the possible variables used during the processing. Figure 3 shows the object-oriented variable tree structure that can be programmed into the Simulator easily.

1.7. during the development of the system, a scenario-based database will be developed that can help decision-making on Waste Generation Management, Proliferation Resistance, Throughput Capabilities, Facility Requirements, and possibly Cost Benefit analysis. The selected database is MS ACCESS and will be interfaced through the TRPSEMPro package.

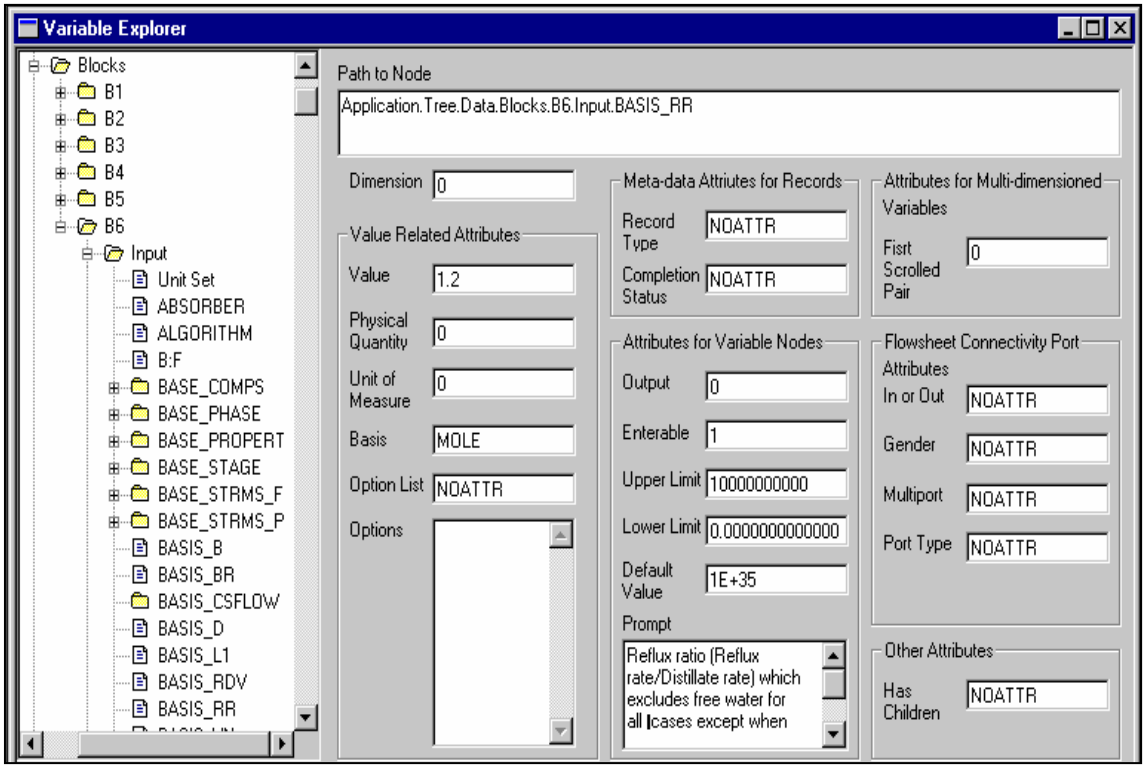

Figure 3 Variable tree structure defined by the ASPEN-PLUS package.

2. Requested by the ANL researchers, the NCACM will setup remote access connection for communication and further study of ASPEN-PLUS package.

3. System Design – identify connecting components from the Aspen Plus package

   3.1. The Aspen Plus Windows user interface provides the function using an ActiveX Automation Server. The ActiveX technology enables an external Windows application to interact with Aspen Plus through a programming interface using a language such as Microsoft's Visual Basic. Since the TRPSEMPro was coded by MS.NET package that can be bridged to the exposed server objects through the COM object model.

   3.2. Since the Aspen Plus process developed by the ANL can be sensitive in its nature, the development of the Aspen Plus Simulator (AspenSim) will be built to use those Aspen Plus components to access the inputs and outputs of the process without revealing process details.

   3.3. Since the ANL is currently working on the process development. Details related to the inputs and outputs will not be available for few more months. Therefore, the NCACM is identifying useful components for handling inputs and outputs. Figure 4 shows a normal process to setup the Aspen Plus sample run case. Each block represents a group of data required by the system. The left-hand side blocks (with the orange color code) are the required parameters while the right-

hand side blocks (with the gray color code) are optional parameters. The input variables within the Data Browser can be viewed as a tree structure shown in Figure 5.

3.4. Aspen Plus also provides an optimization package. The NCACM team will research its capability and compare it with those optimization tools embedded in our TRPSEMPro package.

4. The NCACM allocated a serer-level station for housing ASPEN-PLUS and is working on setting up the remote access connection for ANL researchers.

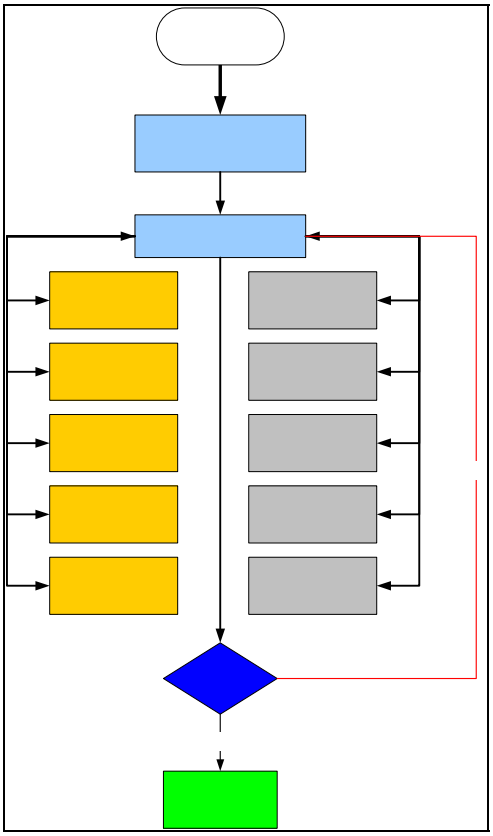

Figure 4 Conceptual steps to construct flowsheet using Aspen Plus package.

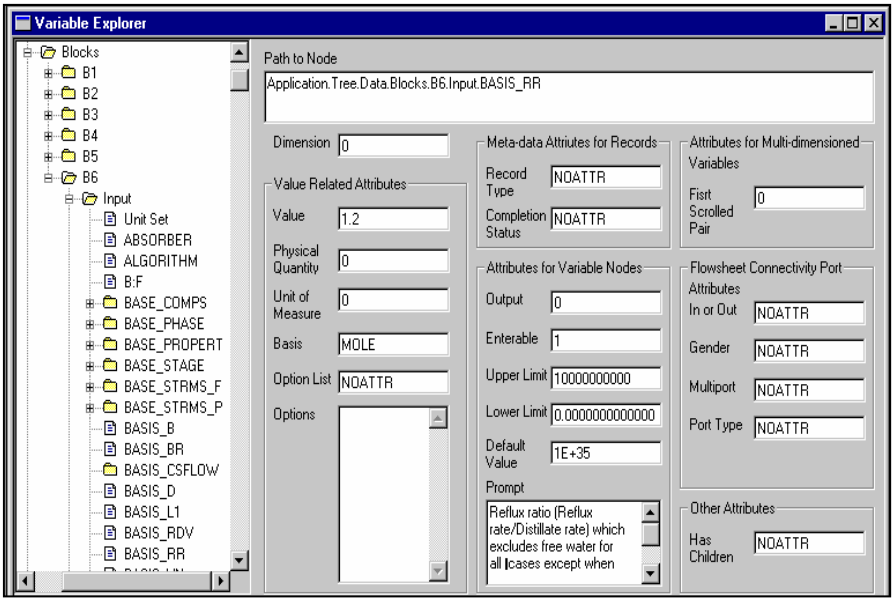

Figure 5 Variable tree structure defined by the ASPEN-PLUS package.

5. TRPSEMPro package improvement – since the package will play a critical role during the system integration, more efforts were placed on modifying program bugs during this month. A summarized items of the improvement are:

    1.1. To simplify the setup procedure, the environmental variable setup uses to define the SEM_PATH was eliminated (changed to “AppPath = Application.StartupPath” from “AppPath =System.Environment.GetEnvironmentVariable("SEM_PATH")”).

    1.2. For a faster and effective debugging processing, the “Multiple Run” module has been rewritten. The default value for executing “Multiple Run” module is set to “Single Run”.

    1.3. As pointed out by the program testing team from the Argonne National Laboratory (ANL), a proper color scheme is required for identifying input data sufficiency. Property dialog box and its coloring scheme associated with the “Stream” category were modified and implemented for such purpose.

    1.4. For clarifying feeding identities while constructing the flowsheet, the program was modified to combine the "Section Letter" and the “Feed Letter" within the flow box. The “Section Letter” is designed to increase by one letter whenever a new “Section” is added, though the values can be overridden by the user under certain special scenarios. The default “Flow Letter” are set to the following as instructed by the ANL:
        - Organic In = X,
        - Aqueous Out = W

- Organic Out = P
- Aqueous In = NULL

1.5. Few incorrect data storage in the EXPORT file have been identified and eliminated. For example, the stage_Efficiency problem in EXPORT file was incorrect and was modified.

6. System Design – identify connecting components from the Aspen Plus package

6.1. The NCACM has allocated a workstation for housing ASPEN-PLUS and has setup up a remote desktop connection for the ANL researchers.

6.2. The purpose for this connection has two folds

- The workstation will be used for familiarizing the ASPEN-plus and constructing basic system analysis cases that can be used for the testing scenarios for the NCACM team.

- Both the ANL and the NCACM teams will use this workstation to identify required parameters for connecting the ASPEN-plus to the TRPSEMPro package. Since the ASPEN-plus was designed with the object-oriented concepts. The exploration of the tree structure has been initialized and will continuously identify the parameters during the next few months.