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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, 2005

Yitung Chen
University of Nevada, Las Vegas, yitung.chen@unlv.edu

Sean Hsieh
University of Nevada, Las Vegas, hsiehht@nscee.edu

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

Quarterly Progress Report
01/01/05- 03/31/05

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

Graduate Students:
- Mr. Mathew Hodges, M.S. Graduate Student, (Mechanical Engineering)
- Mr. Kenny Kwan, M.S., Graduate Student, (Computer Science)

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

Major tasks can be divided into two parts – development of middleware associated with TRPSEMPro and processing modeling using ASPEN-Plus.

1. Development of middleware in TRPSEMPro

1.1. ANL discovered several new non-fission product cation and anion needed to be added into the interface. The new component interface is shown in Figure 1. The changes involved both the code modification on the TRPSEMPro package and the AMUSE macros.

1.2. Prior to fully utilize the optimization module provided by ASPEN-Plus process model, the current TRPSEMPro is required to adjust D value, based on each component within each section, for critical simulation convergence. A new interface shown in Figure 2 was created. The modification involved more fundamental change on the TRPSEMPro code. The D value was designed as a section-related factor that sets to zero initially for simplicity.

1.3. More error handler was implemented. Error-prompted message box contents and EfforInfor.log file format were continuously modified for better identifying the origin of errors. Error message will also be recorded if aqueous and/or organic feed do not have a feed letter

1.4. The team has added an organic flow procedure validation code for identifying a greater-than-zero organic flow rate into the first section and greater-than-zero organic flow out of the last section. Modification of the multiple-run counter was made. The updated TRPSEMPro will force to calculate flow rate prior to the AMUSE simulation run.

2. **Process Model using ASPEN Plus package**

2.1. The NCACM has identified a new graduate assistant, Mr. Matthew Hodges, to work on the chemical process part. He works on creating chemical separation progress using the ASPEN-Plus. The developed process will be passed onto Mr. Kenny Kwan to identify the exposed programming objects. He started to setup up flowsheet with heat exchangers, multiple column options, reactor options, pressure changers, mixers/splitters, and material streams in both liquid and vapor phases.

2.2. The object identification and program communication are undertaking during this quarter.

2.3. Both the ANL and the NCACM teams are using the remote desktop connection for the ASPEN-plus access. The NCACM will need more chemical process input from the ANL once the basic programming components are identified.

2.4. Created several preliminary process models and worked with Mr. Kenny Kwan to successfully enable VB object call and manipulate processes inputs with certain given outputs.

2.5. Mr. Matthew Hodges has created simple ASPEN Plus flowsheet process model for demonstration. The demo model simulates a separation of 99% for water and heptane with operating conditions are as follows (as shown in Figure 3) and the simulated results are shown in Figure 4:

- T_{feed} – 100 C
- P_{feed} – 1 bar
- X_{water} - 0.5
- Stagescolumn – 250
- Reflux Ratio - 10.

2.6. Mr. Kenny Kwan has created a simple interface to input and output parameters from the ASPEN-Plus.

3. Dr. Sean Hsieh has presented research results in the Waste Management 2005 (WM05) meeting in Tucson, AZ on February 28.

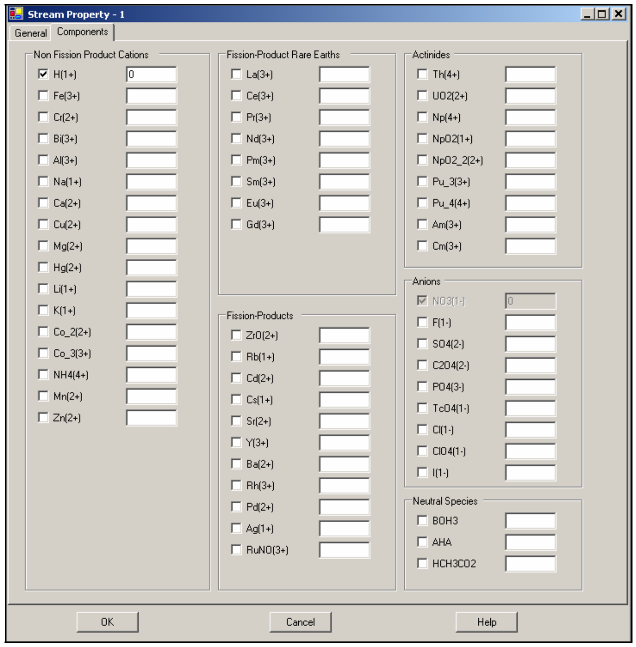

Figure 1 The updated component interface.

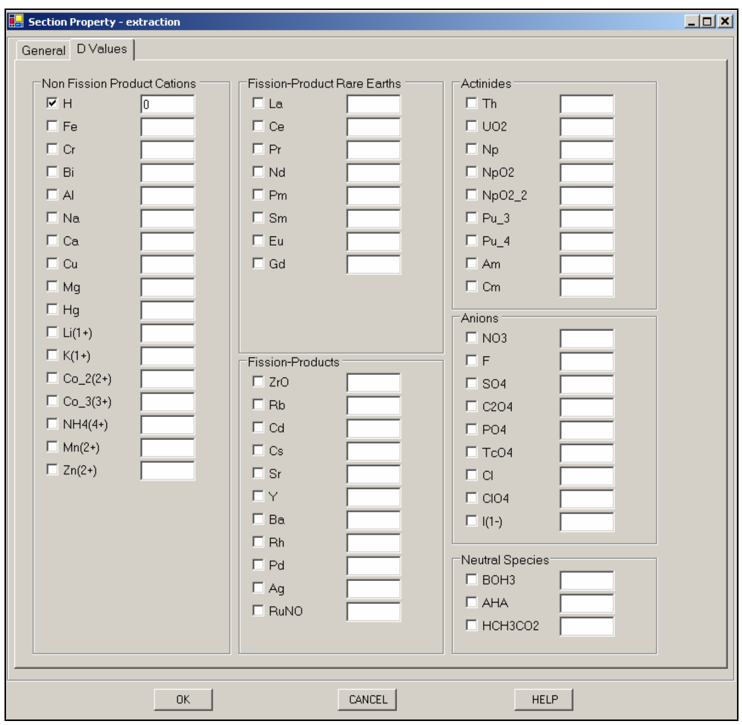

Figure 2 The newly included D value input interface.

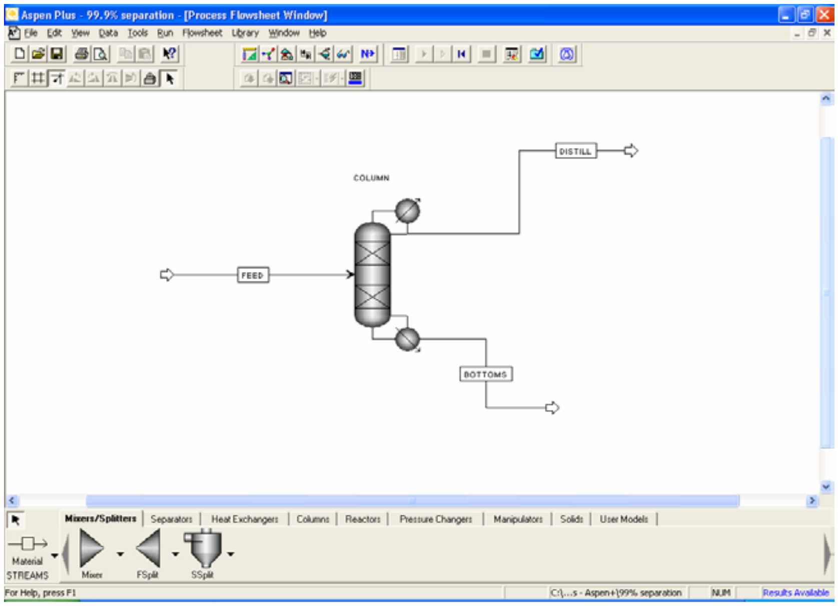

Figure 3 ASPEN-Plus flowsheet.

Display: All streams   Format: GEN_M   Stream Table

	BOTTOMS	DISTILL	FEED	
Temperature C	141.4	99.5	100.0	
Pressure bar	1.000	1.000	1.000	
Vapor Frac	0.000	0.000	0.000	
Mole Flow kmol/hr	100.000	100.000	200.000	
Mass Flow kg/hr	12715.538	1911.771	14627.308	
Volume Flow cum/hr	20.401	2.144	20.765	
Enthalpy MMkcal/hr	-5.718	-6.684	-12.738	
Mole Flow kmol/hr				
3-ETH-01	99.000	1.000	100.000	
WATER	1.000	99.000	100.000	

Figure 4 Simulation results