Development of a Systems Engineering Model of the Chemical Separations Process

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Project Overview

- Two Components
  - Refine AMUSE Code (Ms. Haritha Royyuru)
  - Develop Systems Engineering Model (Mr. Lijian Sun)

- Research Objectives
  - Develop a framework and environment for a systems engineering analysis of the chemical separations system for the AAA program.
  - Establish a baseline systems engineering model from which modifications and improvements can be made.
  - Refine the existing AMUSE program that gives a detailed examination of the UREX process, a critical component of the overall separation scheme.
Argonne National Laboratory
- Chemical Technology Division, Argonne, IL
- Dr. James J. Laidler, Senior Scientist
- Dr. George F. Vandegrift, III, Senior Scientist
  - Dr. Mark Williamson, Chemist
  - Jacqueline Copple, Information Systems Group

Goals
- Work closely with ANL to develop useful graphical module tools for the AAA program
- Educate and train undergraduate and graduate students with regard to system engineering and analysis in chemical separation
What is a System?

- Any process that converts inputs to outputs
- Create outputs based on inputs, the system’s present state
- Definition of state – The current system state and a sequence of subsequent inputs allow computation of the future states of the system

Input → System → Output
System - Example

Input:
- Pedestrians pushing the walk button
- Cars driving over sensors

Output:
- The colored lights in each direction
What is Systems Engineering

Definition 1
- Modeling - Each element of the system and the criterion for measuring performance are described
- Optimization - Adjustable elements are set at values that give the best possible performance

Definition 2
- Requirements Definition
- Conceptual design
- Partitioning of a system into subsystems for other engineering teams to create
- System validation - Ensuring the system works when the subsystems are put together to form the system.
1. Input/Output and Functional Requirement
   - time scale; the set of all admissible inputs over time; the set of all eligible outputs over time; the required functional relationship between the inputs and the outputs.

2. Technology Requirement

3. Input/Output Performance Requirement
   - Specify how well the Input/Output and Functional Requirement is to be met.

4. Utilization of Resources Requirement
   - How well the Technology Requirement is to be met.

5. Trade-Off Requirement (between last two items)

6. System Test Requirement
   - The methods for observing and testing the final system definition
System Engineering - Life Cycle

Concept Development
- Concept Exploration Doc
- System Function Analysis
- System Physical Synthesis

Requirements Development
- Problem Situation Doc
- Operational Need Doc
- The System Req Doc
- System Req Validation

Full Scale Engineering Development

System Development

Test and Integration

Operations, Support, and Modification

Retirement and Replacement
This is what the customer wants, but how will it be measured?

**What? – Customer Demands**

**How? – Quality Characteristic**

**Relationship – Between What and How**

**Correlations – Between “Hows”**

**HOWs vs HOWs**
- Strong positive: 9
- Weak positive: 3
- Weak negative: -3
- Strong negative: -9

**WHATs vs HOWs**
- Strong relationship: 9
- Medium relationship: 3
- Weak relationship: -3

Indication of the importance of that Characteristic in measuring the customer’s satisfaction.
The third QFD chart evaluates the Parts with regard to the Manufacturing Processes. (the goal here is to concentrate on the processes that are ultimately the most important to the customer.)

Charts Chain

• Goal: To satisfy the customer by manufacturing a product that incorporates those things the customer considers important.
Systems Engineering Model of AAA Process

- Apply general systems engineering techniques/tools to complex processes
- What do we hope to accomplish?
  - Development of a tool that allows process changes to be modeled on a system level
    - What impact does one change have on overall process?
  - Mass balance for all process streams
    - Examine changes of input on waste streams
  - Ability to optimize system: cost, waste streams, etc.
  - Detailed models of process components
    - Reactors, electorefining, chopping, separation, etc.
  - Examination of different assumptions on process performance
iSight: Capabilities and Features

A generic software shell - that improves productivity in design process

- Couple simulation code from multiple disciplines
- Easy to set up design problems
- DOE(Design of Experiments) - study and explore design space
- Optimization
  - Combine the best features of existing optimization technologies
  - Can use a technique or a combination of techniques
- Distributed Processing and Parallel Execution
- Solution Monitor
What Process is to be Modeled?

AMUSE Code

- Spent LWR Fuel
  - Chop-Leach LWR Fuel Assemblies
    - Separate U from TRU and FP (UREX process)
    - Prepare U for Disposal or Storage
      - Disposal as LLW
  - Waste Treatment (metal and ceramic forms)
    - FP: fission product
    - TRU: transuranic elements
    - LWR: light water reactor
    - ATW: accelerator transmutation of waste
    - HLW: high-level waste
    - LLW: low-level waste

- ATW Fuel Material Preparation
  - Fuel Fabrication (Metal)
  - Transmutation Assembly Fabrication
    - Fuel Assay
    - ATW Core/Blanket
      - ATW Fuel TRU Separations (Pyro-B)
      - ATW Fuel TRU Separations (Pyro-A)
        - FP Extraction (Pyro-A)
        - Waste Treatment (metal and ceramic forms)
          - TRU, FP
    - Cladding Hulls, FP, Zr
      - Spent ATW Fuel Cooling
        - Chop ATW Fuel

- FP Extraction (Pyro-B)
  - FP Extraction (Pyro-A)
    - FP: fission product
    - TRU: transuranic elements
    - LWR: light water reactor
    - ATW: accelerator transmutation of waste
    - HLW: high-level waste
    - LLW: low-level waste

Hulls & Remaining FP

Tc, I

Tc Targets

I Targets
AMUSE Code - Development Activities

- AMUSE Code a stand-alone tool for the analysis of the UREX process (Uranium Extraction)
- Ms. Haritha Royyuru working on updating this tool
  - User friendly interface tool
  - Visual Basic interface
- AMUSE written within Excel spreadsheet by ANL
  - Graphical output
  - User Friendly/Simple
  - Presently work on AMUSE centers on Interface design
iSight: Problem Setup

- Launch any of iSight interfaces
- Set up and run a design problem

**Task Manager**

- Couple simulation programs
- Specify their execution sequence

- Visual means to monitor the optimization
  - Process: tables and graphs

**Process Integration**

**Problem Definition**

**Solution Monitor**

- Provide problem formulation info to
  - Specific design parameter
Problem Definition

- Parameters
  - Design variables - Which will be perturbed by the optimizer;
  - Objectives - Which will be maximized or minimized during optimization;
  - Constraints - Define the limits, or boundaries, of your design space;
  - Objective function - A weighted sum of all of the parameters designated as objectives in design problem;
  - Feasibility - Indicates $\text{Objective} = \sum W_i * X_i / SF_i$ of the current design point with respect to previous ones.
Example – AMUSE (UREX) Integration
Example - AMUSE (UREX) Integration
Example - AMUSE (UREX) Integration
Optimization - Technique

• Numerical Optimization Techniques
  - ADS-Based Techniques
    • Exterior Penalty
    • Modified Method of Feasible Directions
    • Sequential Linear Programming
  - Generalized Reduced Gradient – LSGRG2 (solving constrained non-linear optimization problems)
  - Hooke-Jeeves Direct Search Method
  - Method of Feasible Directions – CONMIN
  - Mixed Integer Optimization – MOST
  - Sequential Quadratic Programming – DONLP
  - Sequential Quadratic Programming - NLPQL

• Exploratory Techniques

• Expert System Techniques
For combining the multiple optimization techniques

- **Coarse-to-Fine Search**
  - Typically involves using the same optimization technique more than once
- **Establish Feasibility, then search Feasible Region**
- **Exploitation and Exploration**
- **Complementary Landscape Assumptions**
- **Procedural Formulation**
- **Rule-Driven**
Status of Research

- AMUSE training was held on October 9\textsuperscript{th}
- Software structure is currently being studied and reviewed
- Other possible implementations such like MATLAB and SPARK are currently being investigated
- Integration with systems engineering of software tasks is currently being studied and defined
- “Known” systems will be used to test the developed systems analysis
- Parametric studies will be used
- All unit operations will be defined
- Development environment will be developed
- User will be able to examine all waste streams
- Interface with numerous process models will be generated
- Optimization (local and global) will be studied
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