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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.

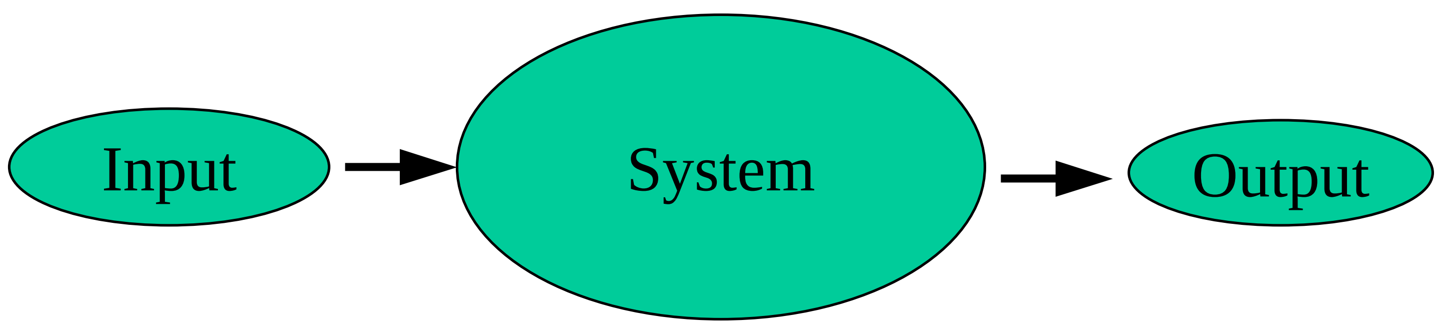
National Laboratory Collaborators

- *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

Project Description – Systems Engineering Approach

What is a System?

- Any process that convert 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



System - Example

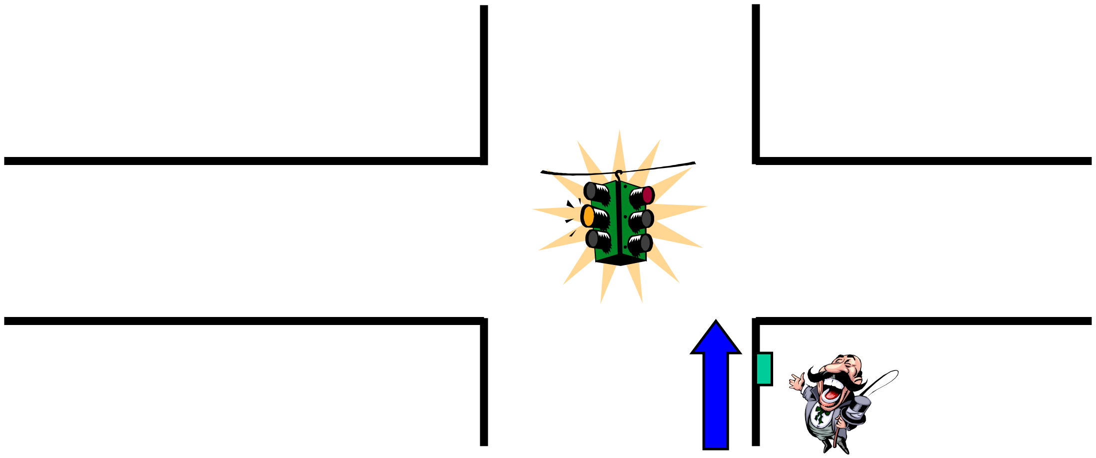
Traffic Light Controller At a Street Intersection

Input:

- Pedestrians pushing the walk button
- Cars driving over sensors

Output:

- The colored lights in each direction



Systems Engineering

What is Systems Engineering

Definition1

- 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

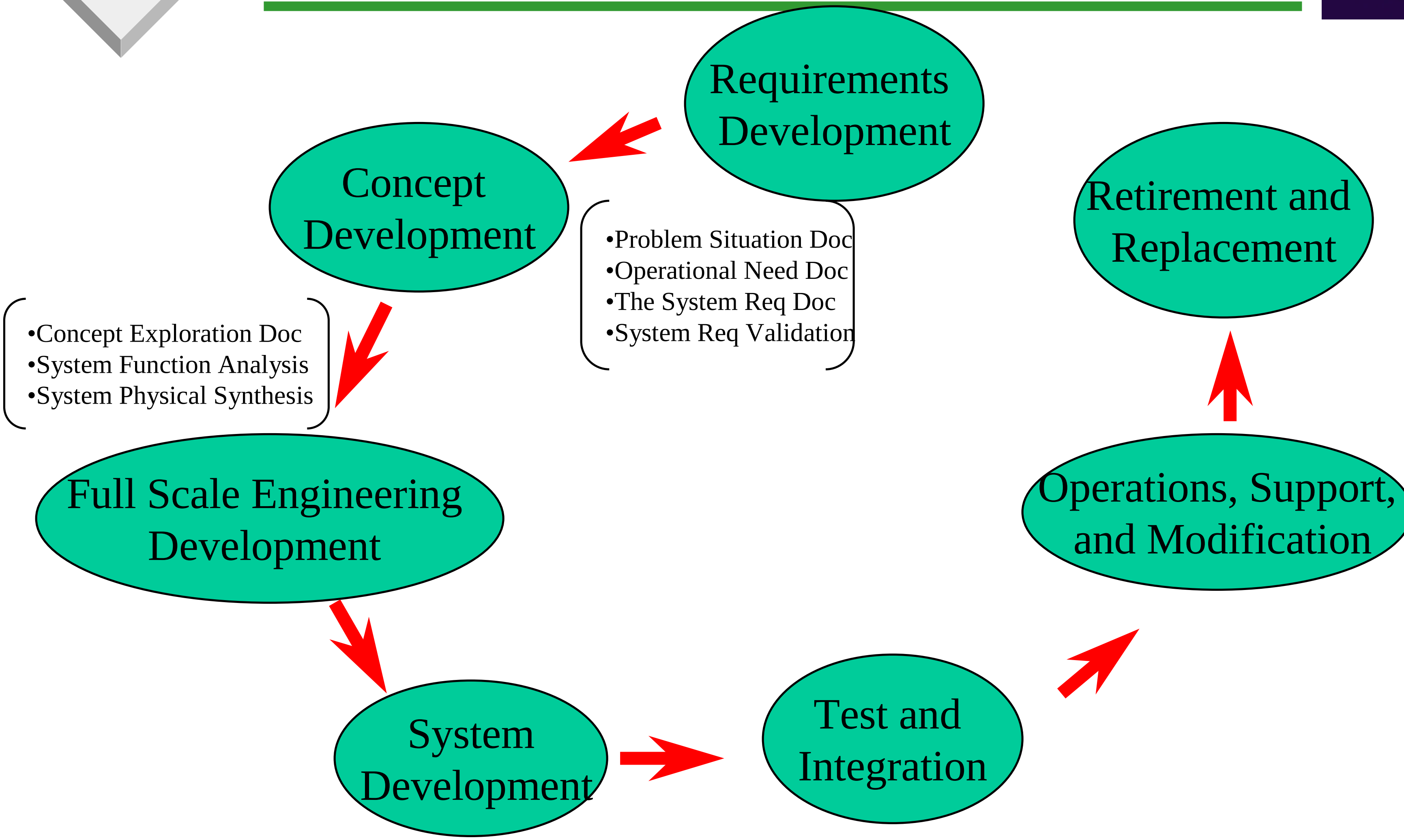
Definition2

- 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.

System Engineering - *System Requirements*

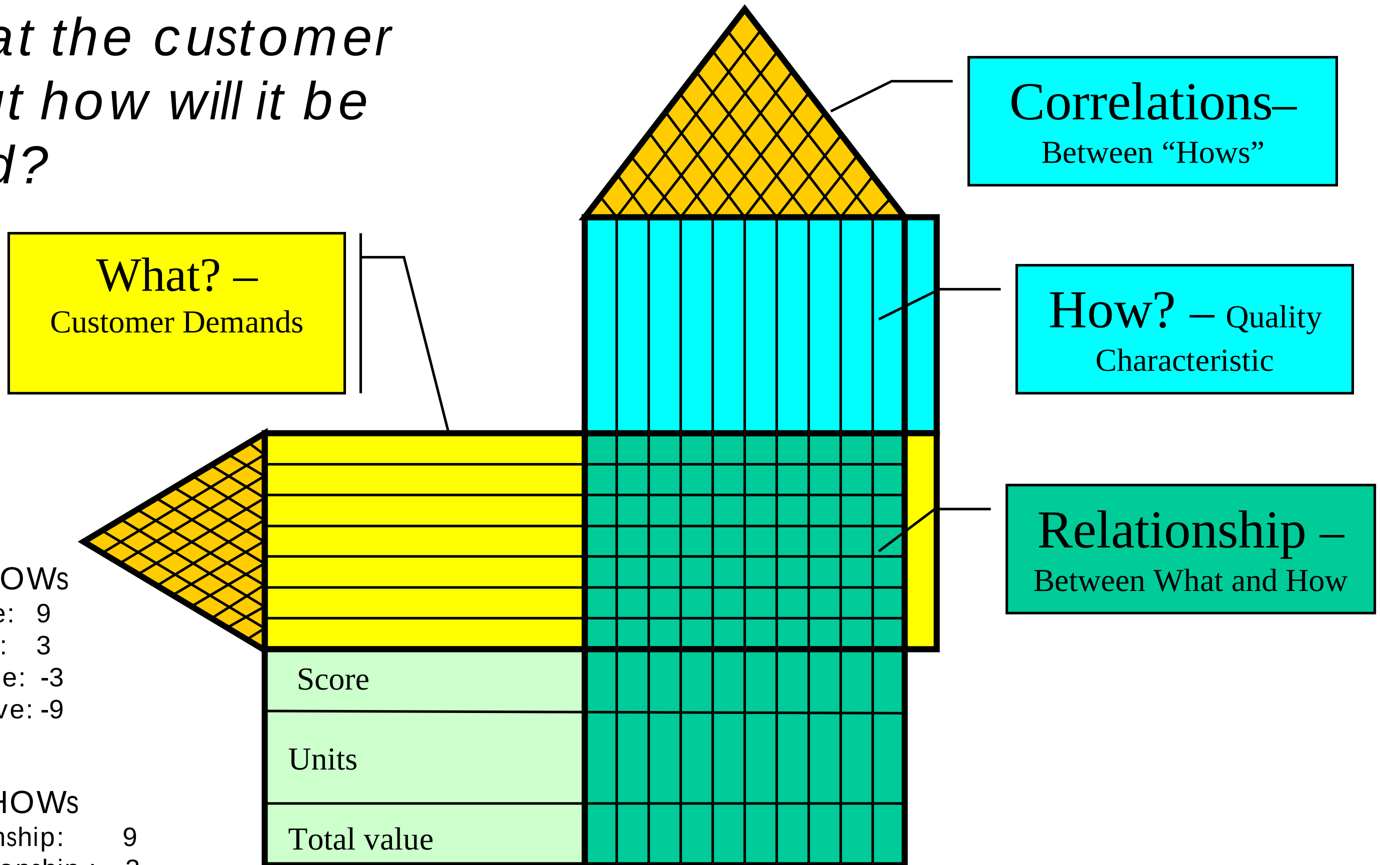
1. Input/Output and Functional Requirement
   - *time scale; the set of all admissible inputs over time; the set of all eligible outputs over time; the required functional relationship between the inputs and the outputs.*
2. Technology Requirement
3. Input/Output Performance Requirement
   - *Specify 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*



House of Quality

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



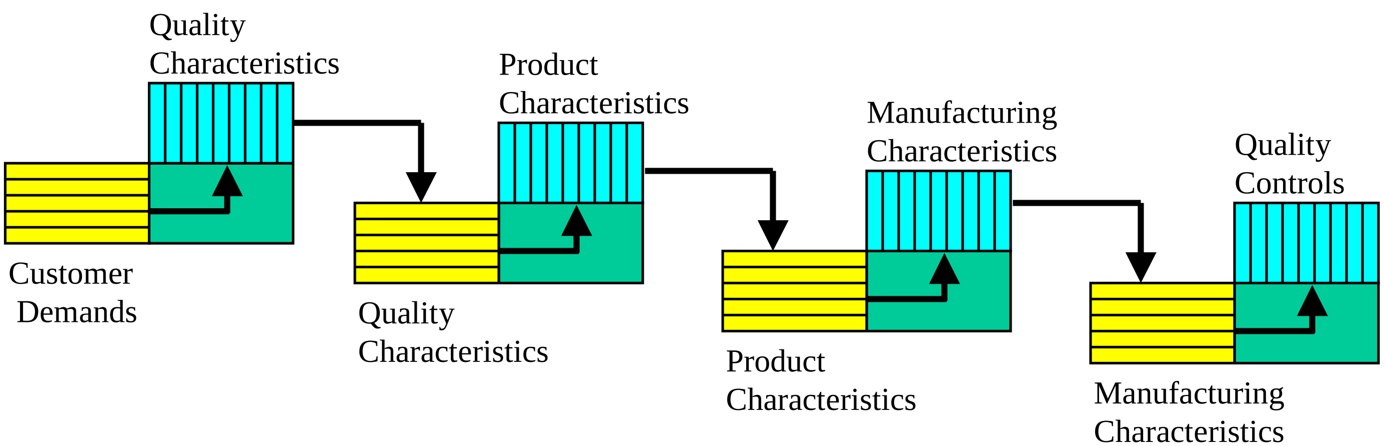
HOWs vs HOWs
Strong positive: 9
Weak positive: 3
Weak negative: -3
Strong negative: -9

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

House of Quality – Cont.

- *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

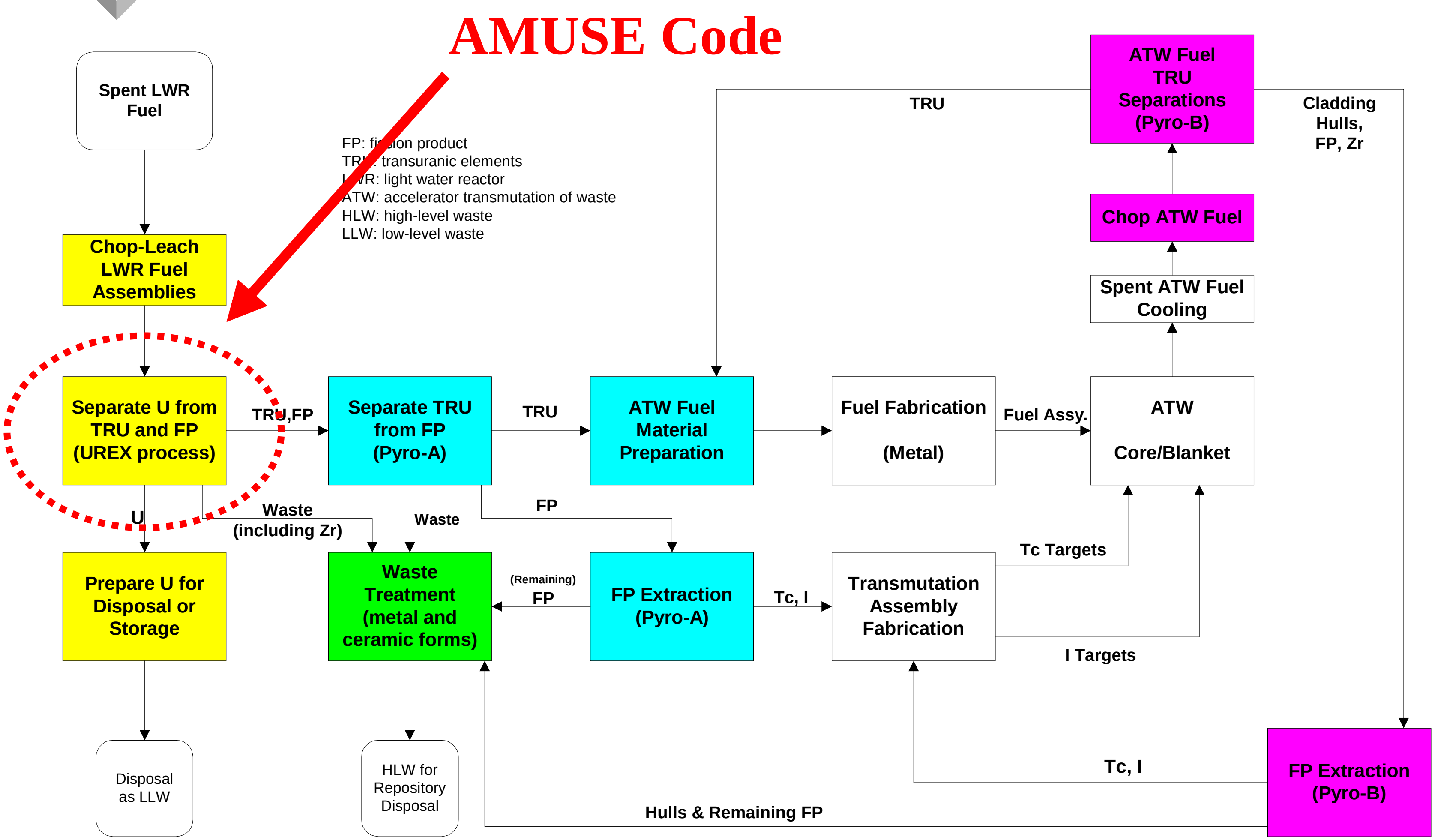
- *Apply general systems engineering techniques/tools to complex processes*
- *What do we hope to accomplish?*
  - Development of a tool that allows process changes to be modeled on a system level
    - What impact does one change have on overall process?
  - Mass balance for all process streams
   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

iSight: Capabilities and Features

A generic software shell - that improves productivity in design process

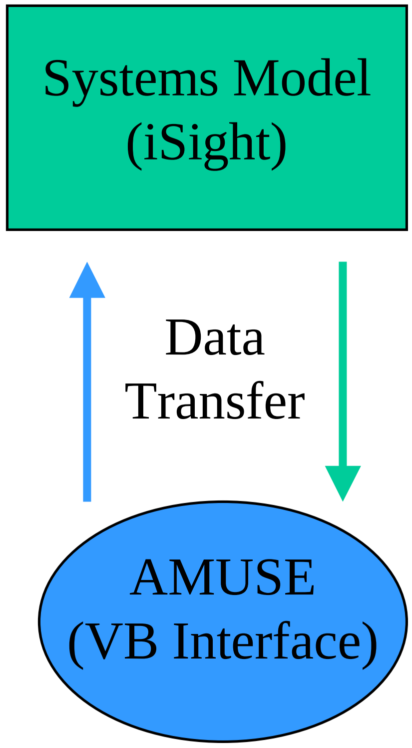
- Couple simulation code from multiple disciplines
- Easy to set up design problems
- DOE(Design of Experiments) - *study and explore design* space
- Optimization
  - Combine the best features of existing optimization technologies
  - Can use a technique or a combination of techniques
- Distributed Processing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

What Process is to be Modeled?



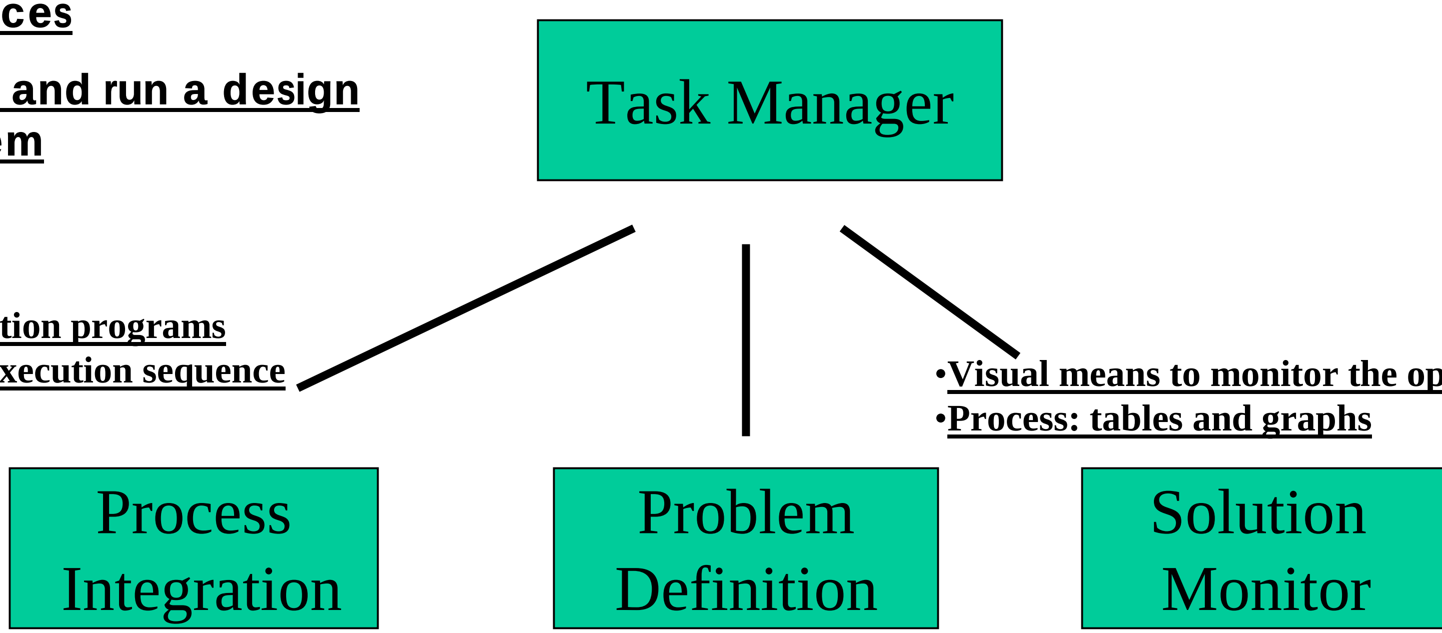
AMUSE Code – Development Activities

- *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

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



- **Couple simulation programs**
- **Specify their execution sequence**

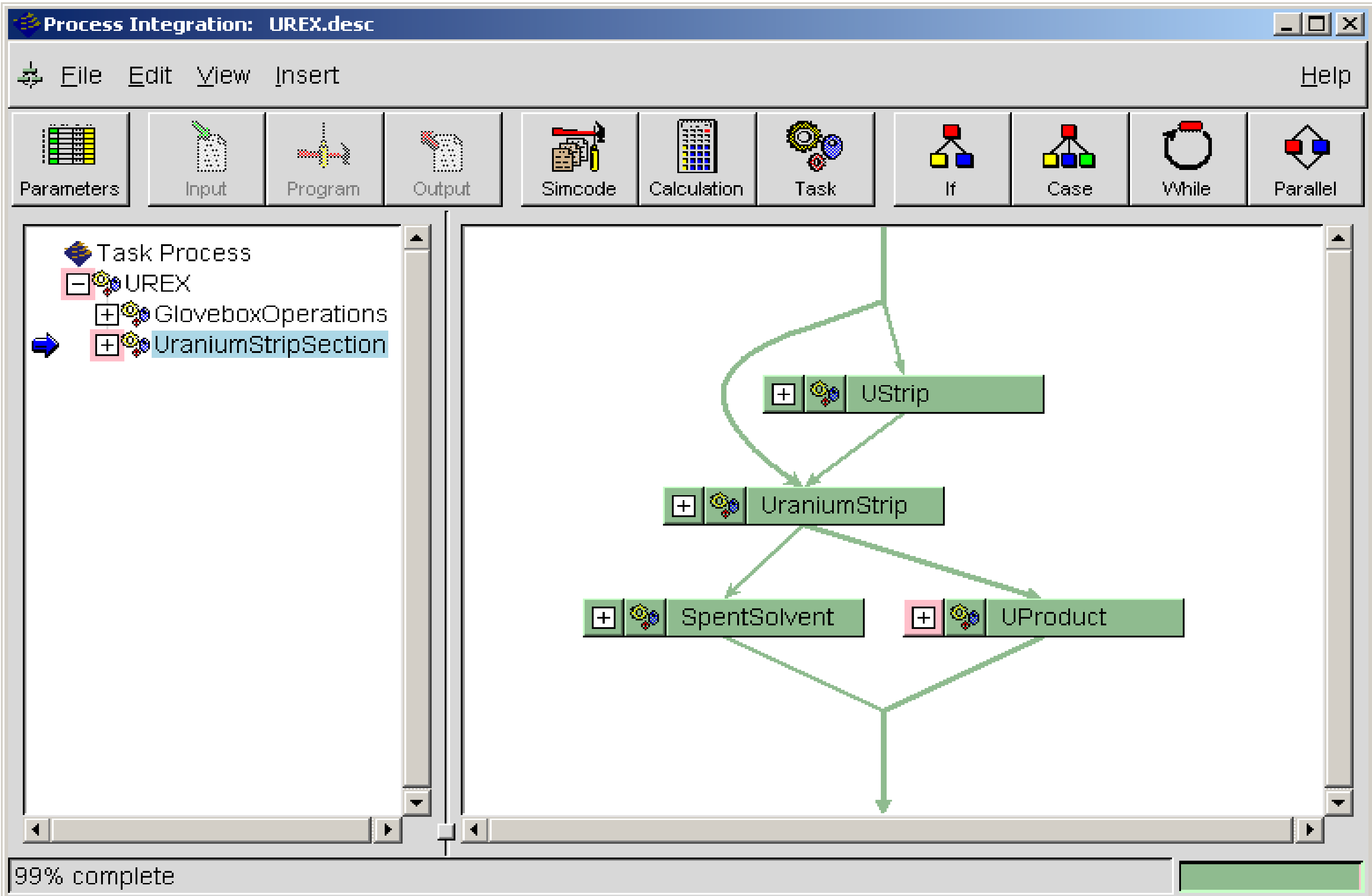
- **Visual means to monitor the optimization**
- **Process: tables and graphs**

- **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 – Indica $Objective = \sum W_i * X_i / SF_i$ of the current design point with respect to previous ones

Example – AMUSE (UREX) Integration



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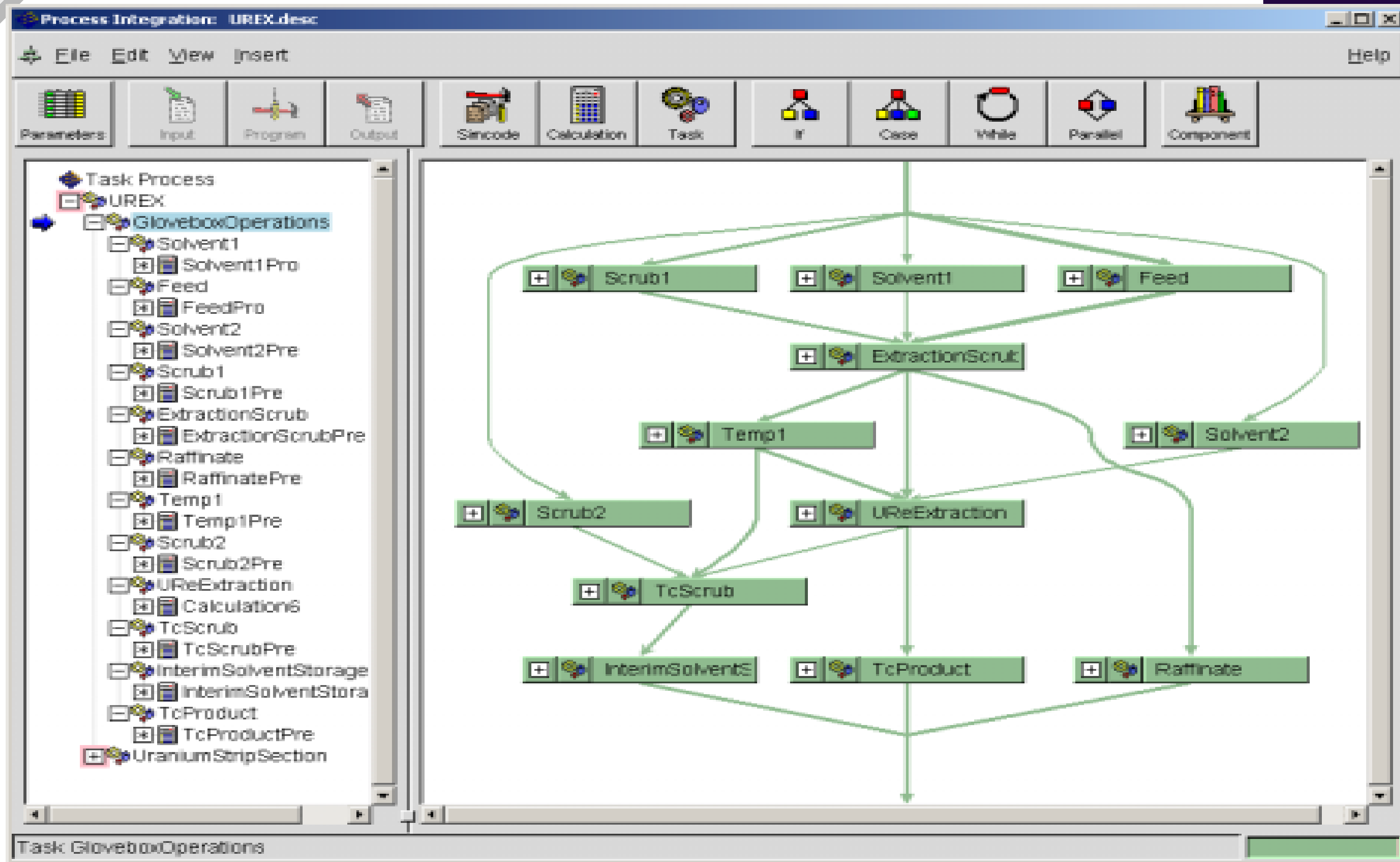
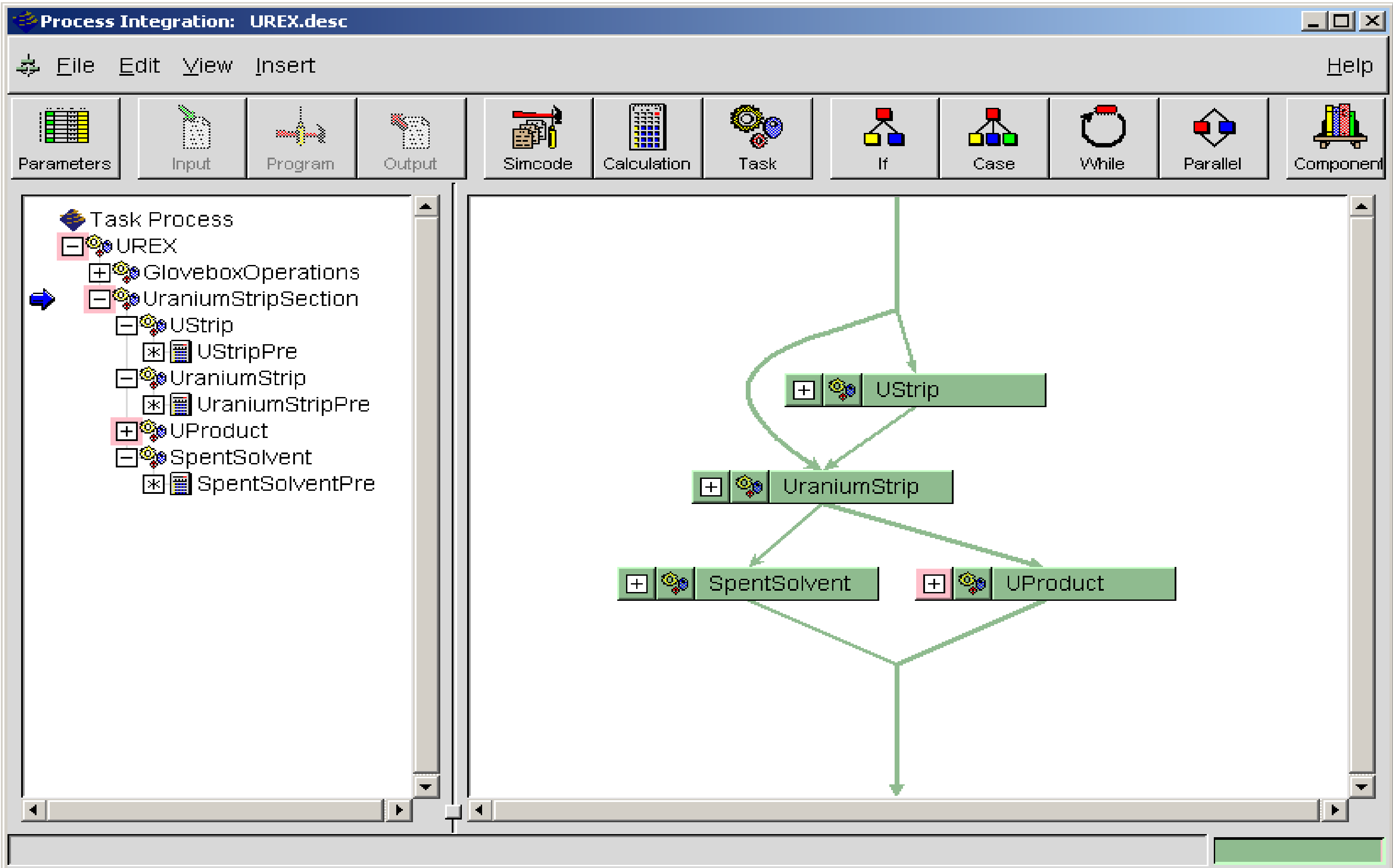


Example – AMUSE (UREX) Integration



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*

Optimization - Strategies

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 9th*
- *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*

Acknowledgements

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