Development of a systems engineering model for chemical separation process

Lijian Sun
University of Nevada, Las Vegas

Follow this and additional works at: https://digitalscholarship.unlv.edu/rtds

Repository Citation
Sun, Lijian, "Development of a systems engineering model for chemical separation process" (2003). UNLV Retrospective Theses & Dissertations. 1565.
https://digitalscholarship.unlv.edu/rtds/1565
DEVELOPMENT OF A SYSTEMS ENGINEERING MODEL
FOR CHEMICAL SEPARATION PROCESS

by

L. Jian Sun

Bachelor of Science, Mechanical, 1995
Hebei University of Technology, Tianjin, P.R.China

Master of Science, Mechanical, 2001
Hebei University of Technology, Tianjin, P.R.China

A thesis submitted in partial fulfillment
of the requirements for the

Master of Science Degree in Mechanical Engineering
Department of Mechanical Engineering
Howard R. Hughes College of Engineering

Graduate College
University of Nevada, Las Vegas
December 2003
The Thesis prepared by

LIJIAN SUN

Entitled

DEVELOPMENT OF A SYSTEMS ENGINEERING MODEL FOR CHEMICAL SEPARATION PROCESS

is approved in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE IN MECHANICAL ENGINEERING

Examination Committee Chair

Dean of the Graduate College

Examination Committee Member

Examination Committee Member

Graduate College Faculty Representative
ABSTRACT

Development of a Systems Engineering Model for the Chemical Separation Process

by

Lijian Sun

Dr. Yitung Chen, Examination Committee Chair
Associate Professor of Department of Mechanical Engineering
University of Nevada, Las Vegas

This thesis is concerned with the efforts to develop a general-purpose systems engineering model software TRPSEMPro that can be used to improve productivity in the design process. Different features of TRPSEMPro will be presented in this thesis. First, Systems Engineering technology is presented, followed by the exposition of different numerical optimization technologies and DOE (Design of Experiments) study technologies. Second, the detailed software process, Object-Oriented Analysis and Design (OOA&D) for the TRPSEMPro is presented. All the design data models are expressed by using Unified Modeling Language (UML).

AMUSESimulator is another software package which has been designed and implemented in order to serve as a bridge between AMUSE Macro, developed by ANL, and systems engineering model, TRPSEMPro. The design process for AMUSESimulator is elaborated in this thesis.

1 TRPSEMPro - Transmutation Research Program System Engineering Model Project
The topics in this thesis also include SQL Server Database, XML, DOE techniques and optimization techniques. Several study cases which apply the developed systems engineering model to solve typical design problems are demonstrated.
# TABLE OF CONTENTS

ABSTRACT..............................................................................................................iii

LIST OF FIGURES...................................................................................................v

ACKNOWLEDGEMENTS..............................................................................................vii

CHAPTER 1 INTRODUCTION AND BACKGROUND .............................................1
  1.1 Project Background – TRP Program and Chemical Separation Process ...... 1
  1.2 Objective............................................................................................................4
  1.3 Capabilities and Features of the Developed Systems Engineering Model Package. 5
  1.4 The Structure of this thesis ..............................................................................6
  1.5 Software Implementation Tool .......................................................................6

CHAPTER 2 SYSTEM ENGINEERING .....................................................................8
  2.1 Introduction to System Engineering.................................................................8
    2.1.1 Why Do We Need System Engineering?...................................................8
    2.1.2 What is a System?.....................................................................................9
    2.1.3 Definition of Systems Engineering............................................................10
  2.2 Introduction to Modeling..................................................................................10
    2.2.1 Why Must We Model Things?..................................................................10
    2.2.2 Definition of a Model................................................................................12
    2.2.3 Principles of Modeling..............................................................................12
  2.3 Implementation of System Engineering Techniques for Chemical Separation
     Process ................................................................................................................13
    2.3.1 System Identification and Familiarization ...............................................13
    2.3.2 Model Isolation and Boundary Setting ....................................................14
    2.3.3 Analysis of System Equations ...................................................................15
  2.4 The System Architecture for TRPSEMPro......................................................17
  2.5 TRPSEMPro’s Role in the Design Cycle .........................................................18

CHAPTER 3 DOE STUDY AND OPTIMIZATION .............................................20
  3.1 Design of Experiments (DOE) Study .............................................................20
    3.1.1 Purposes of Design of Experiments (DOE) Study ...................................20
    3.1.2 DOE Study Techniques .........................................................................21
  3.2 Optimization.....................................................................................................25
    3.2.1 Introduction to Optimization ....................................................................25
    3.2.2 Formal Elements of Optimization Problem ...........................................26
    3.2.3 Category of Optimization Problem ............................................................28
    3.2.4 Basic Mathematical Concepts ..................................................................28
    3.2.5 Numerical Techniques for Nonlinear Programming Problem ...............32
LIST OF FIGURES

Figure 1-1  Overall Chemical Separations System for TRP Program ..................... 1
Figure 1-2  UREX Process ................................................................................. 3
Figure 1-3  Project Tasks .................................................................................... 5
Figure 2-1  Definition of System ....................................................................... 9
Figure 2-2  Schematic representation of the process for model development .... 13
Figure 2-3  UREX Process ................................................................................. 15
Figure 2-4  System Architecture for TRPSEMPRO ........................................ 17
Figure 2-5  Multi-Program Design Cycle .......................................................... 19
Figure 3-1  Full-Factorial Study ...................................................................... 22
Figure 3-2  Parameter Study ............................................................................. 22
Figure 3-3  Central Composite Design ............................................................. 24
Figure 3-4  Category of Optimization Problem ................................................. 28
Figure 3-5  Generic Algorithm for Unconstrained Optimization ..................... 33
Figure 3-6  Algorithm - Random Walk .............................................................. 34
Figure 3-7  Algorithm - Conjugate Gradient (Fletcher-Reeves) Method .......... 35
Figure 3-8  Algorithm - Davidon-Fletcher-Powell Method (DFP) .................... 37
Figure 3-9  Algorithm - Augmented Lagrange Multiplier (ALM) method ...... 39
Figure 4-1  Phases of Software Process ............................................................. 41
Figure 4-2  OOA&D Roadmap ........................................................................ 44
Figure 4-3  OOA&D Approach for Obtaining Domain Classes ...................... 45
Figure 4-4  Use Case for System Engineering Model ....................................... 46
Figure 4-5  Sequence Diagram for System Engineering Model ....................... 47
Figure 4-6  Use Case for Model Integration ...................................................... 48
Figure 4-7  Sequence Diagram for ModelIntegration ........................................ 49
Figure 4-8  Use case for StudyPlanBuilder ....................................................... 50
Figure 4-9  Sequence Diagram for StudyPlanBuilder ....................................... 51
Figure 4-10 Use case for SolutionViewer ......................................................... 52
Figure 4-11 Sequence diagram for SolutionViewer ......................................... 53
Figure 4-12 System Architecture .................................................................... 55
Figure 4-13 Static Diagram for System Engineering Data Model .................... 56
Figure 4-14 Sequence Diagram for Composite Design Pattern in DataModel ... 57
Figure 4-15 Static Diagram for ModelIntegration ............................................. 57
Figure 4-16 Static Diagram for StudyPlan ......................................................... 58
Figure 4-17 Static Diagram for SolutionViewer ................................................ 58
Figure 5-1  Relationship among System Engineering Model, AMUSESimulator, and AMUSE Macro ................................................................. 59
Figure 5-2  Framework of AMUSESimulator .................................................... 61
Figure 5-3  Identify Objects in UREX Process (Provided by ANL) .................... 61
Figure 5-4  Architecture of AMUSESimulator ................................................ 63

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Figure 5-5  Static Diagram for Main Data Models for AMUSESimulator .............. 63
Figure 5-6  Static Diagram for FSGraphics ..................................................... 64
Figure 5-7  Observer Design Pattern Applied to AMUSESimulator ................... 65
Figure 5-8  Diagram for the Structure of Database Design ............................... 66
Figure 5-9  Dialog for Loading Flowsheet from Database ............................... 66
Figure 5-10  Whole Flowsheet is Selected by Default .................................. 67
Figure 5-11  Property Dialog for Flowsheet .................................................. 68
Figure 5-12  Section is Selected ..................................................................... 69
Figure 5-13  Property Dialog for Section ...................................................... 70
Figure 5-14  Stream is Selected ..................................................................... 70
Figure 5-15  Property Dialog for Stream ...................................................... 71
Figure 5-16  Utility Module - Database Viewer .............................................. 72
Figure 6-1  The Main Interface of SystemManager ........................................ 74
Figure 6-2  Insert a Calculation Model ......................................................... 75
Figure 6-3  Define the Input and Output Parameters .................................... 75
Figure 6-4  Input the Formula in the Graphical Way ..................................... 76
Figure 6-5  Input the Formula in the Tabular Way ...................................... 76
Figure 6-6  Display of Newly Added Calculation Model in SystemManager .... 77
Figure 6-7  Problem Definition - Definition of Constraint, Objective and Design Variable ....................................................................................................................... 79
Figure 6-8  Specify Study Plan - Optimization with Random Walk Technique ...... 79
Figure 6-9  DOE Study Plan: Factor Specification ....................................... 80
Figure 6-10  DOE Study Plan: Factor Interaction Specification ...................... 80
Figure 6-11  DOE Study Plan: Design Matrix Display .................................... 81
Figure 6-12  Optimization Study Plan: Choose Optimization Techniques ........ 81
Figure 6-13  Optimization Study Plan: Specification of Detailed Information .... 82
Figure 6-14  Add Defined Study Plan to the Calculation Model .................... 82
Figure 6-15  Configure Graph Page ............................................................... 84
Figure 6-16  Configuration of Chart: Select Chart Type ................................ 84
Figure 6-17  Configuration of Chart: Select Parameter of Interest ................... 85
Figure 6-18  Configuration of Table: Select Parameter of Interest ................... 85
Figure 6-19  Choose the Defined Study Plan ................................................ 86
Figure 6-20  Result Display: By Way of Graph Page .................................... 87
Figure 6-21  Result Display: In a Separate Window ...................................... 87
Figure 6-22  Rosenbrock (Banana) Function ............................................... 88
Figure 6-23  Conjugate Gradient Method: Solution Display in Chart Form ....... 90
Figure 6-24  Conjugate Gradient Method: Solution Display in Tabular Form .... 90
Figure 6-25  Random Walk Method: Solution Display in Tabular Form .......... 91
Figure 6-26  Random Walk Method: Solution Display in Chart Form .............. 91
Figure 6-27  Problem Definition Dialog ....................................................... 92
Figure 6-28  ALM Method: Solution Display in Tabular Form ....................... 93
Figure 6-29  Glovebox Phase of UREX Process ........................................... 94
Figure 6-30  Integration of Chemical Separation Process: Glovebox Phase of UREX Process ................................................................................................................................. 95
ACKNOWLEDGEMENTS

The financial support funded by Transmutation Research Program - University Participation Program (TRP-UPP)/Department of Energy (DOE) is highly appreciated. The technical supports associated with the background information and chemical separation process model information were provided by Argonne National Laboratory-East.

I would like to express my deepest gratitude to my advisors, Dr. Yitung Chen and Dr. Hsuan-Tsung (Sean) Hsieh, who gave me inspiration and guidance throughout my graduate studies at the University of Nevada, Las Vegas. I would also like to give my sincere appreciation to my committee members, Dr. Robert F. Boehm and Dr. Yahia Baghzouz, for their precious time and advice for my research. Special thanks also go to Dr. George Vandegrift and Ms. Jackie Copple of Argonne National Laboratory for their knowledge and support.

I appreciate all the colleagues in our research center, NCACM (Nevada Center for Advanced Computation Method), for sharing many valuable research ideas.

I owe great love to my parents who have made many sacrifices over the years to get me to this point, and my wife, Ms. Xiuling Wang, who has shared all the wonderful and difficult moments with me and will forever.

Thanks also to the many who have helped me through my quest for higher education.
CHAPTER 1

INTRODUCTION AND BACKGROUND

This chapter will introduce the project background information and then give a brief overview about this thesis’s content.

1.1 Project Background – TRP² Program and Chemical Separation Process

![Diagram of Overall Chemical Separations System for TRP Program]

The United States is embarking on a national program to develop accelerator transmutation of high-level radioactive waste (ATW) as part of the Transmutation

² TRP - Transmutation Research Program
Research Program (TRP) project at its national laboratories. Through the Program TRP, the U.S. joins international efforts to evaluate the potential of partitioning and transmutation along with advanced nuclear fuel cycles. Transmutation means nuclear transformation that changes the contents of the nucleus (protons and/or neutrons). The TRP is a developing technology for the transmutation of nuclear waste to address many of the long-term disposal issues. An integral part of this program is the proposed chemical separations scheme. Figure 1.1 shows a block diagram of the current process as envisioned by Argonne National Laboratory (ANL) researchers (Gregory R. Choppin, 1999; G. F. Vandegrift, 1992; Gregory R. Choppin, 2002).

Nearly all issues related to risks to future generations arising from long-term disposal of such spent nuclear fuel is attributable to ~1% of its content. This 1% is made up primarily of plutonium, neptunium, americium, and curium (the transuranic elements) and long-lived isotopes of iodine and technetium created as products from the fission process in power reactors. When transuranics are removed from discharged fuel destined for disposal, the toxic nature of the spent fuel drops below that of natural uranium ore (that was originally mined for nuclear fuel) within a period of several hundred years.

Figure 1.1 depicts the fuel cycle scheme in which the transuranic elements and long-lived fission products from Light Water Reactor (LWR) spent fuel are sent directly to an accelerator-driven subcritical reactor for transmutation. Other schemes under consideration involve intermediate critical reactor steps; this would result in major changes in the design, development and analysis of separations systems. Systems engineering would enhance the ability to respond with such changes.
Removal of plutonium and other transuranics from material destined for geologic disposal also eliminates issues related to long-term (centuries) heat management within geologic environments. The removal of neptunium, technetium, and iodine render negligible the possibility of radioactive material penetration into the biosphere far in the future. Finally, removal of plutonium negates any incentive for future intrusion into repositories driven by overt or covert recovery of material for nuclear proliferation.

The complete process considers existing LWR spent fuel, separation processes, fuel fabrication, transmutation, disposal as a low-level waste (LLW), and the reprocessing of fuel after transmutation. This is an involved process that can be varied in a number of ways. Any proposed change to the process can have impacts on the fuel design, amount of waste generated by the process, number of cycles through the reactor, etc. In a nuclear growth scenario, the introduction of advanced thermal reactor designs will almost certainly result in changes in separations system requirements that must be met with optimized systems.

Figure 1-2 UREX Process
The separation process can be systematically identified as a group of blocks that have specific separation functions. One block's effluent flows into another block as input. Each block has its process target. For a complex process like separation process, a systems engineering model is critical for designing and refining the whole chemical separation process.

However, most of the blocks (subprocesses) are still under development or revision. The research now is focused on the Uranium Extraction process (UREX). The process is for separation of TRU (Transuranic) elements from the dissolved spent fuel as shown in Figure 1-2. The process needs to report 95% of technetium (Tc) and 99.9% of uranium consistent to a separate effluent. The U/Tc-free TRU/fission product (fp) stream is then fed to PYRO-A process. The recovered uranium is purified for Low Level Waste (LLW) disposal while recovered technetium is used for transmutation of targets.

1.2 Objective

The research is to develop a system engineering modeling software package, TRPSEMPro (Transmutation Research Program System Engineering Model Project), that allows researchers to construct process blocks, connect blocks and analyze the chemical separation process in a systematic and optimized ways. Features of the work are listed as below:

Integrate chemical separation process into systems engineering model

Identify core functions of system engineering model for the current or selected separation process scenarios

Develop and implement software tool that allow to build system model and optimize the partial or entire chemical separation process

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Demonstrate software and model capabilities with various pre-defined scenarios

Due to the availability of the process modules, this research only demonstrates the system engineering model involved interfacing with the UREX process that is calculated by Argonne Model for Universal Solvent Extraction (AMUSE) software package. The ANL developed AMUSE code, based on the Microsoft Excel macros, is identified as a standalone external module and kept intact. A midware-like Flowsheet-Simulator is developed to interact with AMUSE package. The similar communication pathway can be built while more extraction modules, such as Pu/Np or Cs/Sr extraction modules are available.

![Figure 1-3 Project Tasks](image)

**Figure 1-3 Project Tasks**

### 1.3 Capabilities and Features of the Developed Systems Engineering Model Package

- 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 either single technique or a combination of techniques
• Provide Solution Viewer to view the design running results.

1.4 The Structure of this thesis

Chapter 2 is focused on identifying modules in chemical separation process and on building system engineering model based on the criteria; Chapter 3 will introduce some core functions required for system engineering, such as Design of Experiment (DOE) and optimization; Chapter 4 discusses software design for TRPSEMPro. That includes Model-View-Observer pattern and data structures. It also zooms into the integration module or interface between existing extraction process software and system engineering model; Chapter 5 introduces the interface module required for connection of any existing module with the system engineering package. Current research demonstrates the interface module to the AMUSE code; finally, since the sensitive nature of the UREX process, the provided AMUSE code is a simplified version that blocks the actual calculation of certain parameters. Chapter 6 provides some testing scenarios that primarily demonstrate the capabilities of the design software rather than the accurate simulation results from chemical separation process software AMUSE.

1.5 Software Implementation Tool

Software Implementation Tools include the following four parts:
Microsoft™.Net - Microsoft™.Net architecture allows programmers to develop components using a number of different programming languages, including C#, C++, Eiffel, J#, and Visual Basic. The resulting components (called “assemblies” by Microsoft) can use each other, regardless of the source language used to construct each one. Microsoft™.Net is the main programming language used in the software development (Deitel 2002, Microsoft 2002, Lowell Manuer 2002 and et al.).

XML (eXtensible Markup Language) - With the growing popularity of XML, XML Schema is being widely used to describe data. XML is intended to be a self-describing data format, allowing authors to define a set of element and attribute names that describe the content of a document. XML Schema was chosen as the method for describing the structure of system engineering model, also, XML Database is used to store all the run time data for AMUSE module (Kurt Cagle 2000, Mark Graves 2002, R. Allen Wyke 2002 and et al.).

SQL Server 2000 database

UML (Unified Modeling Language) – UML is a graphical notation for expressing object-oriented designs. It is a melding of the notations of Booch, Rumbaugh, Jacobson, Wirf-Brock, and Herel among others. The official UML standard is managed by the Object Management Group consortium of companies (www.omg.org), and requires hundreds of pages to formally specify. Design models in this thesis are expressed by using UML (Booch 1999, James Rumbaugh 1999 and et al.).
CHAPTER 2

SYSTEM ENGINEERING

This thesis is primarily concerned with the development of system engineering model, therefore it seem to be appropriate to give some background information about systems engineering at this initial stage. First, the definitions of system, systems engineering, and the need for systems engineering are discussed; Second, the concept and necessity for modeling are included. Third, the applications of system engineering techniques are discussed.

2.1 Introduction to System Engineering

2.1.1 Why Do We Need System Engineering?

Is there a real need or is it just some academic exercise to appear knowledge? To answer this question, let us first look at the three common reasons for project failure and disasters.

(1) Complexity. This is certainly one of the main causes of system problems. Brooks, often viewed as the father of software engineering and one of the great software philosophers (if such things exists), identifies two main types of complexity that exist in almost all systems (software and otherwise) (Brooks 1995): essential complexity and accidental complexity. Essential complexity is in the essence of the system. This means that it is an inherent part of a system and, as such, can not be eliminated. Accidental
complexity is complexity that creeps into the system by accident. It is caused by accident or, to put it another way, by error, but it is possible to do something about it. (2)

Communications. A lack of communication or inefficient communication will contribute to project failure. The channels of communication may exist at an organization level, may exist between different teams within a single organization, between different resources, such as hardware, software, networks, protocols, etc.; may exist between different levels of management. (3) Lack of understanding.

These problems do not simply occur during the design and implementation of a project, but may appear at any phase in the project’s life cycle. Therefore, the way in which we approach systems engineering must be applicable at any point in the project life cycle rather than simply focusing on a single phase or phase activity. This will turn out to be a fundamental requirement for system engineering

2.1.2 What is a System?

What do we actually mean by a system? A common misconception is that a system is simply a product that may be delivered at the end of a project. However, this is not the case. A system is any process that converts inputs to outputs (Andrew P. Sage 2000). A system creates outputs based on inputs, over which it has no direct control, and the system’s present state. The current system state and a sequence of inputs allow computation of the future states of the system.

Figure 2-1 Definition of System
2.1.3 Definition of Systems Engineering

The term "systems engineering" means different things to different people. Here are three common definitions:

Definition 1: John G. Truxal, former Dean of Engineering at Brooklyn Polytechnic Institute, says (William 1992), "System Engineering includes two parts: modeling, in which each element of the system and the criterion for measuring performance are described; and optimization, in which adjustable elements are set at values that gives the best possible performance.

Definition 2: A division manager at Hughes Aircraft Company defined systems engineering as performing (William 1992): (a) requirements definition, (b) conceptual design, (c) partitioning of a system into subsystems (guidance, propulsion, etc) for other engineering teams to create, and (d) system validation, i.e., ensuring the system works when the subsystems are put together to form the system. Particular attention must be paid to the interface between the subsystems.

Definition 3: System Engineering is concerned with defining and implementing an approach to solving problems, while managing complexity and communicating over the entire lifetime of a project (Jon Holt 2001).

2.2 Introduction to Modeling

2.2.1 Why Must We Model Things?

In order to justify the need for models, the easiest is to look at a number of simple examples. The examples used here are based on those defined by the modeling master, Grady Booch (Booch G. 1999).
Behind Booch’s three examples, the kennel, the house and the office block, there is a very serious and fundamental point.

Nobody in their right mind would attempt to build an office block with basic DIY skills. In addition, there is the question of resources, and not only in terms of the materials needed. In order to build an office block, you would need the knowledge to access the necessary human resources, plenty of time and plenty of money. The strange thing is that many people will approach building a complex system with the skills and resources of a kennel-builder, without actually knowing if it is a kennel, house or office block. When contemplation any complex system, you should assume that it will be, or has the potential to turn into, an office block building. Do not approach any project with a ‘kennel’ mentality. If you approach a project as if it were an office block and it turns out to be kennel, you will end up with a very well-made kennel that is the envy of all canines. If, however, you approach a project as if it were a kennel and it turns out to be an office block, the result will be pure disaster!

One of the reasons why it is so easy to misjudge the size and complexity of a project is that, in many cases, many elements of the system will not be tangible or comprehensible. Projects fail for many different reasons; there are three main themes, which have already been discussed: complexity, lack of understanding and communication. However, many projects do succeed. One reason is that they avoid, or minimize, the aforementioned problems due to effective modeling.

There are still other reasons for modeling. Here is the list for the purpose of modeling:
(1) visualize a system; (2) specify a system; (3) serve as a template for creation; (4) in order to document decisions made throughout the project.
2.2.2 Definition of a Model

The definition of a model from Booch (Booch G 1999) is that: a model is defined as simplification of reality that is created in order to better understand the system under development, as we cannot comprehend complex systems.

2.2.3 Principles of Modeling

Booch (Booch G 1999) identifies four principles of modeling that are deemed crucial for successful and consistent modeling: the choice of model, the level of abstraction, connection to reality and independent views of the system.

The choice of model: it will have a profound influence on how a problem is approached. Approaching a problem the right way can make a job much simpler and will be quicker than adapting the wrong approach;

Abstraction of the model: ‘abstraction’ refers to the level of detail of a model. The point to be made here is that any model will require different levels of abstraction to be represented; otherwise the model will have little chance of being correct;

Connection to reality: One problem with modeling is that, according to the definition, models simplify reality. This means that some information must be lost somewhere along the line, which can cause problems. Therefore, it is vital to know both how the model relates to real life and how far it is divorced from real life. From a practical point of view, initial models tend to have quite a loose connection to reality and, as these models evolve, they get closer and closer to reality. The final connection to reality will be at the point when the model actually becomes reality, which is when the model is implemented or constructed based on the model.
Independent views of the same system: A good model requires views modeled from different vantage points and requires views that represent different levels of abstraction. One crucial point that must be made here, however, is that each of these independent views must be consistent with one another, or, to put it another way, they must integrate correctly.

2.3 Implementation of System Engineering Techniques

for Chemical Separation Process

Implementation of system engineering model is an approachable solution to solve complex process, such as chemical separation. To help user to build a model on a system level and perform system analysis, we will develop a software tool that allows building system models through user-friendly interface. System engineering model itself includes analysis tools, such as parameter study, optimization, and Design of Experiments (DOE) study, especially designed for the chemical separation process. Schematically, the model development approach is shown in Figure 2-2.

![Figure 2-2 Schematic representation of the process for model development](image)

2.3.1 System Identification and Familiarization

The beginning of any system study is Block 1 in Figure 2-1, System Identification and Familiarization. Often, to a simple system, identifying the essential components of
the system that collectively undergo the cause and effect action associated with the system is obvious, such as the illness (the output) that results when a person (the system) consumes toxic food or water (the input). However, the identification and isolation of other systems, such as a study of the causes of inflation where the general system is the world economic system, is undoubtedly complex, diverse, and presents a serious modeling challenge.

For this project, clearly defining the process flow sheet is a critical first step. Figure 1-1 shows one presentation of the proposed process.

2.3.2 Model Isolation and Boundary Setting

All of the present work centers on the three center blocks of Figure 2-1. The involved TRP chemical separation process can be systematically identified as a group of blocks that have specific separation functions: existing LWR spent fuel, separation processes, fuel fabrication, transmutation, disposal as a low-level waste (LLW), and the reprocessing of fuel after transmutation as listed in Figure 1-1. One block’s effluent flows into another block as input. Each block has its process target. Task in ANL is to develop each individual model for these chemical separation processes. Most of the blocks (sub processes) are still under development or revision. So far, research is focused on the Uranium Extraction process (UREX) block as shown in Figure 2-3.

The UREX process is for separation of TRU (Transuranic) elements from the dissolved spent fuel as shown in Figure 2-3. The process needs to report 95% of Tc and 99.9% of U to a separate effluent. The U/Tc–free TRU/Fp stream is then fed to PYRO-A process. The recovered Uranium is purified for low level waste (LLW) disposal while recovered technetium is used for transmutation of targets.
2.3.3 Analysis of System Equations

Each of the Process Blocks as shown in Figure 1-1 will have a set of equations or relationships to model the transport of mass through that process. These relationships may be relatively simple, or complex computer codes like the AMUSE code. While chemical engineering systems are getting more complex, the process becomes more difficult to analyze mathematically. The development of Systems Engineering Model allows industries to model the process more quantitatively and to study the interactions between subsystems and performance of the model under the influence of various design parameters. Systems engineering is a multidisciplinary function dedicated to controlling design so that all elements are integrated to provide an optimum, overall system. Detailed process flowchart will be elaborated in Chapter 3.

Developing a systems engineering model of the overall chemical separation process would be beneficial to analyzing complex interactions between proposed process changes. The model will evolve over several years to incorporate all process steps and to improve process modules as more knowledge is gained.
The graphical representation of the systems engineering model, which includes its inputs and outputs and possible feedback, is a very useful tool in the initial modeling and formulation stage of a system study. The act of graphically and schematically portraying the system is conducive to accurate identification and improved understanding of what inputs interact with the system components and how these interactions produce the outputs anticipated. It is in the graphical representation stage of modeling that the system investigator or apprentice could be as thorough and critical of all the known or anticipated system factors as possible. The investigator or apprentice could attempt to detail the system and individually “componentize” the system elements as much as possible.

Frequently, a very valuable aid in the initial identification of the inputs and outputs and various subsystems of a given system is to graphically model the overall system, including explicit designation of all subsystems and internal inputs and outputs. The powerful influence of visual and special conception and recognition of the model in a graphic format can be very revealing and productive for both model analysis and synthesis.

To UREX process, the visual definition can be performed in program module AMUSESimulator, and user can actively define inputs/outputs of this process module in graphic format, the detail information about UREX process will be discussed in Chapter 5. The definition of inputs/outputs is the key to a proper mass balance.

Block diagrams, signal-flow graphs, and organizational diagrams, as graphical modeling tools have been developed in this project. Several major specific engineering system identification and modeling techniques will be examined in detail in Chapter 3.
The basic single-input, single-output model has been widely used and justified as an excellent beginning model for many systems. For the present process, some process steps may allow a simple model to be used for the initial process evaluation.

2.4 The System Architecture for TRPSEMPro

In TRPSEMPro, design problems are specified, and simulation codes from multiple disciplines are coupled into a system model description file written in XML. After a description file is created, the user can use the application interface to set up, monitor, and analyze a design run.

![System Architecture for TRPSEMPro](image)

Figure 2-4 System Architecture for TRPSEMPro

A few critical components are required during the system modeling, input/output parameters, relationships among blocks (such as sequence of execution of extraction processes), system analysis, and process monitoring.

The designed system model includes four main parts as shown in Figure 2-4.
System Manager – System Manager is the main application interface, from where a user can launch any of the application interfaces. The System Manager allows the user to set up and run a design problem.

Model Integration – Model Integration enables user to couple simulation programs to system engineering model and specify their execution sequence. Model Integration provides a GUI that acts as a front end for creating an system engineering model description file written in XML language.

StudyPlan – StudyPlan provides a convenient means to provide problem formulation information to specific design parameters, the allowing user to control information in a specific problem. Techniques such as Optimization and Design of Experiments (DOE) are available in Study Plan.

Solution Viewer – Solution Viewer provides a visual means to monitor the optimization process as it moves through the design space. Solution Viewer provides several tables and graphs that can be used to view the runtime changes.

2.5 TRPSEMPro’s Role in the Design Cycle

The typical practice design engineers employ in either product or process design is known as the design-evaluate-redesign cycle. As shown in Figure 2-5, this cycle involves the iterative processing of input files, the running of one or more simulation programs, and the analysis of output files. The cycle continues until the design criteria are reached and the best design (one that satisfies the customer requirements and meets design constraints) is chosen by the design engineer.

The role of TRPSEMPro is to automate the design-evaluate-redesign cycle, eliminate the human intervention bottleneck. In Figure 2-5, the Study Plan (a single, self-contained
design unit with its own parameters, optimization strategy) drives the automation of the cycle. By eliminating costly human intervention, TRPSEMPRo lets the designer refocus valuable engineering time on design analysis and selective refinement of the design process.

TRPSEMPRo system can be harnessed to execute more than just computer simulation programs. TRPSEMPRo can automate the execution of a sub model (independent models that are invoked by the main model) to support a hierarchical, multilevel design problems.

Figure 2-5 Multi-Program Design Cycle
CHAPTER 3

DOE STUDY AND OPTIMIZATION

In this chapter, knowledge about DOE Study and optimization are discussed. After integrating of all the individual models into the system engineering model, these two technologies are the core to do the system analysis.

3.1 Design of Experiments (DOE) Study

Design Of Experiment (DOE) – it is a general term that refers to any of the many formal methods available for setting parameter values in a set of experiments.

3.1.1 Purposes of Design of Experiments (DOE) Study

The purpose of DOE study is listed as follows:

- To assess design variable impact
- To identify significant design variable interactions
- To analyze a design space and provide a rough estimate of an optimal design, which can be used as a starting point for numerical optimization
- To screen a large set of design variables for a subsequent numerical optimization (design space reduction)

To do the DOE study, you should know the following things:

- Parameters you want to study (i.e., the parameters that may impact performance/quality)
- Number of experiments or trials you can afford to run
- Output quantities of interest (i.e., those that in some way represent the performance/quality of the product)
- Overall goal of the study (i.e., design variable screening, estimation of an optimal design, response surface approximation)

3.1.2 DOE Study Techniques

Several techniques about DOE study have been studied, these include Full-Factorial, Parameter Study, Data File, Orthogonal Arrays, Central Composite and Latin Hypercubes (Liu 1993, Guri 1994).

Full-Factorial Design: In a full-factorial study, the user specifies the values at which to study each parameter and then to run all combinations of these values. If $i$ is the number of factors and $n$ is the number of levels or values at which to study each factor, then a total of $\prod n_i$ designs must be evaluated.

Parameter study: The Parameter Study allows one parameter at a time to be studied at different values, with all other parameters held at their base value. After a parameter has been studied at each of the specified values, it is restored to its base value for studying the other parameters. It is similar to a sensitivity analysis. In this case, if $i$ is the number of parameters and $n$ is the number of levels at which to study each parameter, then the total number of designs to be evaluated is $1 + \sum n_i$, where the one additional evaluation is for the baseline design.

The table below illustrates the difference between the Full-Factorial Study and the Parameter-Study. In this example, we have three factors – A, B, and C. Each is to be
studied at two levels – 1 or 2. The baseline design values for the parameter study are designated by the level 0.

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

Figure 3-1 Full-Factorial Study

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>2</td>
</tr>
</tbody>
</table>

Figure 3-2 Parameter Study

Data File: With the Data File study, it is possible to analyze design points in a tab- or space- delimited file by associating the columns of the data file with the user specified parameters.

Orthogonal Arrays: The use of orthogonal arrays let you avoid a costly full-factorial experiment in which all combinations of all inputs (or factors) at different levels are studied ($p^n$ for $n$ factors each at $p$ levels), and instead perform a fractional factorial.
experiment. A fractional factorial experiment is a certain fractional subset (1/2, ¼, 1/8, etc.) of the full factorial set of experiments, carefully selected to maintain orthogonality (independence) among the various factors and certain interactions. It is this orthogonality that allows for independent estimation of factor and interaction effects from the entire set of experimental results.

Central Composite Design: Central Composite Design (CCD) is a statistically-based technique in which a 2-level full-factorial experiment is augmented with a center point and two additional points for each factor (called “star points”). Thus, five levels are defined for each factor, and to study n factors using Central Composite Design requires $2^n + 2^n + 1$ design point evaluations. Figure 3-3 shows the Central Composite Design points for three factors.

The center and star points are added to acquire knowledge from regions of the design space inside and outside the 2-level full factorial points, allowing for an estimation of higher-order effects (curvature). The star point(s) are determined by defining a parameter which relates these points to the full-factorial points by:

$$
S_{upper} = b + (u - b) \times a \\
S_{lower} = b - (b - 1) \times a
$$

Where:

$$
b = baseline \ design = lower \ factorial \ point \\
u = upper \ factorial \ point < b < u
$$

Note that:

$$
a < 1, \ star \ points \ are \ inside \ the \ full-factorial \ design \\
a > 1, \ star \ points \ are \ outside \ the \ full-factorial \ design \\
a = 1, \ star \ points \ are \ the \ same \ value \ as \ the \ full-factorial \ levels
$$

(also referred to as face-centered central composite design)
Although Central Composite Design requires a significant number of design point evaluations, it is a popular technique for compiling data for Responses Surface Modeling due to the expense of design space covered, and the higher-order information obtained.

Latin Hypercubes: Another class of experimental design which efficiently samples large design spaces is Latin Hypercube sampling. With this technique, the design space for each factor is uniformly divided (the same number of divisions (n) for all factors). These levels are then randomly combined to specify n points defining the design matrix (each level of a factor is studied only once). For example, the figure illustrates a possible Latin Hypercube configuration for two factors (X1, X2) in which five points are studied. Although not as visually obvious, this concept easily extends to multiple dimensions.

An advantage of using Latin Hypercubes over Orthogonal Arrays is that more points and more combinations can be studied for each factor. The Latin Hypercube technique allows the designer total freedom in selecting the number of designs to run (as long as it...
is greater than the number factors). The configurations, however, are more restrictive using the Orthogonal Arrays.

3.2 Optimization

3.2.1 Introduction to Optimization

One of the primary tasks of the systems engineer is to ensure the optimization of the design process.

Driven by competition, quality assurance, cost of production, and finally, the success of the business enterprise, the subject of optimization is receiving serious attention from engineers, scientists, managers, and most everybody else. Now, optimization is practiced through software programs and requires significant computer resources. The techniques of optimization have not changed significantly in recent years, but the areas of application in professional practice require at least three prerequisites. They include mathematical modeling of the design problem, knowledge of computer programming, and knowledge of optimization techniques.

Optimization can be applied to all disciplines. Qualitatively, this assertion implies multiple decision choices; implicitly recognizing the necessity of choosing among alternatives. In this project, we deal with optimization in a quantitative way which means that an outcome of applying optimization to the problem, design, or service must yield numbers that will define the solution, or in other words, numbers or values that will characterize the particular design or service. Quantitative description of the solution requires a quantitative description of the problem itself. This description is called a mathematical model. The design, its characterization, and its circumstances must be expressed mathematically.
3.2.2 Formal Elements of Optimization Problem

To go further in the area of optimization, the formal elements of the optimization problem must be introduced first. It should be understood that optimization presupposes the knowledge of the design rules for the specific problem, primarily the ability to describe the design in mathematical terms. These terms include design variables, design parameters, and design functions. Traditional design practice, that is, design without regard to optimization, includes all of these elements although they were not formally recognized as such. This also justifies the prerequisite that you must be capable of designing the object if you are planning to apply the techniques of optimization. It is also good to recognize that optimization is a procedure for searching the best design among candidates, each of which can produce an acceptable product.

Design variables are entities that identify a particular design. In the search for the optimal design, these entities will change over a prescribed range. The values of a complete set of these variables characterize a specific design. The number and type of entities belonging to this set are very important in identifying and setting up the quantitative design problem.

Design Parameters, in this thesis, identify constants that will not change as different designs are compared.

Design functions define meaningful information about the design. They are evaluated using the design variables and design parameters. They establish the mathematical model of the design problem. These functions can represent design objective(s) and/or constraints. Design objective drives the search for the optimal design. The satisfaction of
the constraints established the validity of the design. The designer is responsible for identifying the objectives and constraints.

We can assemble the general abstract mathematical model as following:

Minimize:

$$f(x_1, x_2, \cdots, x_n)$$  

Subject to:

$$
\begin{align*}
\begin{cases}
 h_j(x_1, x_2, \cdots, x_n) &= 0 \\
 g_j(x_1, x_2, \cdots, x_n) &= 0 \\
 & \vdots
\end{cases}
\end{align*}
$$  

$$
\begin{cases}
 h_l(x_1, x_2, \cdots, x_n) &= 0 \\
 x_l^i & \leq x_i \leq x_u^i, i = 1, 2, \cdots, n
\end{cases}
$$

Exploiting vector notation the mathematical model is:

Minimize:

$$f(X), [X]_n$$  

Subject to:

$$
\begin{align*}
[h(X)]_e &= 0 \\
[g(X)]_m &= 0 \\
X^{low} & \leq X \leq X^{up}
\end{align*}
$$

The above mathematical model expressed the following standard format of the optimization problem expressed in natural language:

Minimize the objective function $f$, subject to $l$ equality constraints, $m$ inequality constraints, with the $n$ design variables lying between prescribed lower and upper limits.

The search of the optimal solution will depend on the nature of the problem being solved.
3.2.3 Category of Optimization Problem

The category of Optimization Problem is shown in Figure 3-4 (Edwin 1996, Boris 1987).

![Figure 3-4 Category of Optimization Problem](image)

3.2.4 Basic Mathematical Concepts

The basic mathematical elements in the discussion of Nonlinear Programming (NLP) are derivatives, partial derivatives, vectors, matrices, Jacobian, and Hessian (David 1978).

Numerical derivative computation: Many numerical techniques in NLP require the computation of derivatives. The derivative for the single-variable function at any value $x$ is also called slope or the gradient of the function at that point. To two or more independent variables the equivalent concept is the partial derivative. Partial derivative is defined for each independent variable.
The gradient of the function is a vector, and at any point represents the direction in which the function will increase most rapidly. Examining the conventional objective of NLP, minimization of objective function, the gradients has a natural part to play in the development of methods to solve the problem. The gradient is composed of the partial derivatives organized as a vector.

The Jacobian \([J]\) defines a useful way to organize the gradients of several functions. Using three variables and two functions \(f(x, y, z)\) and \(g(x, y, z)\), the definition of the Jacobian is:

\[
[J] = \begin{bmatrix}
\frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \\
\frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} & \frac{\partial g}{\partial z}
\end{bmatrix}
\]  

(3.6)

The first row is the gradient of \([df \ dg]^T\) while the second row is the gradient of \(g\). If the two functions are collected into a column vector, the differential \([df \ dg]^T\) in the functions, due to the differential change in the variables \([dx \ dy \ dz]\), can be expressed as a matrix multiplication using the Jacobian

\[
\begin{bmatrix}
[dx] \\
[dy] \\
[dz]
\end{bmatrix}
= [J] \begin{bmatrix}
[dx] \\
[dy] \\
[dz]
\end{bmatrix}
\]  

(3.7)

Hessian matrix \([H]\) is the same as the matrix of second derivative of a function of several variables. For \(f(x, y)\):
For a function of \( n \) variables \( f(X) \), where \( X = [x_1, x_2, \ldots, x_n]^T \), the gradient is

\[
\nabla f = \left[ \frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n} \right]^T
\]  

(3.9)

The Hessian is

\[
[H] = \begin{bmatrix}
\frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\
\frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2}
\end{bmatrix}
\]  

(3.10)

Taylor's Theorem/Series is a useful mechanism to approximate the value of the function \( f(X) \) at the point \((X_p + \Delta X)\) if the function is completely known at current point \( X_p \) (\( \Delta X \) is the displacement vector),

\[
f(X_p + \Delta X) = f(X_p) + \nabla f(X_p)^T \Delta X + \frac{1}{2} \Delta X^T H(X_p) \Delta X + \ldots
\]  

(3.11)

3.2.4.1 Analytical Conditions for General Optimization Problem:

Optimization problems whose mathematical models are characterized by nonlinear equations are called Nonlinear Programming (NLP) problems. Engineering design problems are mostly nonlinear. Here, a traditionally bottom-up presentation of knowledge for nonlinear optimization will be given as follows (David 1978 and Donald 1986). Unconstrained problems are discussed first followed by constrained problems.
Unconstrained Problem: First-Order Conditions (FOC): FOC are usually regarded as necessary conditions.

\[ \nabla f(X^*) = 0 \quad (3.12) \]

Second-Order Conditions (SOC): SOC are usually regarded as sufficient conditions. It can be inferred that these conditions will involve second derivatives of the function. The SOC is often obtained through the Taylor expansion of the function to second order. If \( X^* \) is the solution, and \( \Delta X \) represents the change of the variables from the optimal value which will yield a change \( \Delta f \), then

\[
\Delta f = f(X^* + \Delta X) - f(X^*) = \nabla f(X^*)^T \Delta X + \frac{1}{2} \Delta X^T H(X^*) \Delta X \quad (3.13)
\]

Since \( \Delta f \geq 0 \) and Equation (3.12), then, \( \Delta f = \frac{1}{2} \Delta X^T H(X^*) \Delta X > 0 \)

Where \( H(X^*) \) is the Hessian matrix (the matrix of second derivatives) of the function \( f \) at the possible optimum value \( X^* \). For the relation in equation to hold, the matrix \( H(X^*) \) must be positive definite.

Equality Constrained Problem:

Minimize \( f(X), [X]_n \) \quad (3.14)

Subject to:

\[
\begin{align*}
[ h(X) ]_p &= 0 \\
X_{low} &\leq X \leq X_{up}
\end{align*}
\quad (3.15)
\]

Lagrange Multipliers method is an elegant formulation to obtain the solution to a constrained problem.
Inequality Constrained Optimization: An inequality constrained problem can be transformed to an equality constrained problem by introducing a slack variable for each inequality constraint, then the solution can be found.

Scaling: Numerical calculations are driven by larger magnitudes. The standard approach to minimize the impact of large variations in magnitudes among different equations is to normalize the relations. In practice this is also extended to the variables. This is referred to as scaling the variables and scaling the functions. Many current software will scale the problem without user intervention.

The presence of side constraints in problem formulation allows a natural definition of scaled variables. The user-defined upper and lower bounds are used to scale each variable between 1 and 0. Therefore,

\[ x_i' = \frac{x_i - x_i'}{x_i'^u - x_i'^l}; x_i' = \text{scaled } i^{th} \text{ variable} \]  \hspace{1cm} (3.16)

\[ x_i = x_i'(x_i'^u - x_i'^l) + x_i'^l \]  \hspace{1cm} (3.17)

3.2.5 Numerical Techniques for Nonlinear Programming Problem

Following sections will illustrate several numerical techniques for multivariable optimization problems which are implemented in our developed software system (Donald 1986, User Guide: Optimization Toolbox for Use With MATLAB 2000). While the unconstrained optimization is not a common occurrence in engineering design, nevertheless the numerical techniques included here demonstrate interesting ideas and also provide the means to solve constrained problems after they have been transformed into an unconstrained one.
3.2.5.1 Unconstrained Optimization

All the algorithms which can be used to solve unconstrained optimization problems are iterative; the iteration takes place by moving along a search direction vector during an iteration. These search directions can be determined in many ways. The different techniques that are presented here primarily differ in how the search direction is established. The remaining elements of the algorithm, except for the convergence/stopping criteria, are the same for almost all of the methods; the generic algorithm can be expressed as shown in Figure 3-5.

![Figure 3-5 Generic Algorithm for Unconstrained Optimization](image-url)
Random Walk Method: Random Walk is called a zero-order method. In this method, the search direction during each iteration is a random direction (Please refer to Figure 6-20, Figure 6-21, Figure 6-25, and Figure 6-26 for examples of using this method).

Choose $X_0$, $N$ (number of iterations)
Set $i = 1$

For each iteration $i$
$S_i = \text{Random vector}$

$X_{i+1} = X_i + \alpha_i S_i$
$\alpha_i$ is determined by minimizing $f(X_{i+1})$

$i = i + 1$

Yes
$i < N$

No
Stop

Figure 3-6 Algorithm – Random Walk

Conjugate Gradient (Fletcher-Reeves) Method: Originally due to Fletcher and Reeves, this method has the property of quadratic convergence because the search directions are conjugate with respect the Hessian matrix at the solution. A quadratic
Choose \( X_0, N \) (number of iterations)
\[ f_0(x) = f(X_0), X_0(x) = X_0 \] (store values)
\( \varepsilon_1, \varepsilon_2, \varepsilon_3 \) (tolerance for stopping criteria)

Yes

\[ i = 1? \]

Yes

\[ S_i = -\nabla f(X_i) \]

\[ \beta = \frac{\nabla f(X_i)^T \nabla f(X_i)}{\nabla f(X_{i-1})^T \nabla f(X_{i-1})} \]
\[ S_i = -\nabla f(X_i) + \beta S_{i-1} \]

\[ X_{i+1} = X_i + \alpha_i S_i \]
\( \alpha_i \) is determined by minimizing \( f(X_{i+1}) \)
\[ X_{i+1}(i) \leftarrow X_{i+1}; f_{i+1} = f(X_{i+1}) \] (Store values)

\[ \Delta f = f_{i+1} - f(i); \Delta X = X_{i+1} - X_i \]

Yes

\[ |\Delta f| \leq \varepsilon_i ? \]

No

Yes

\[ \Delta X^T \Delta Y \leq \varepsilon_i ? \]

No

Yes

\[ i = i+1 \]

No

Yes

\[ \nabla f(X_{i+1})^T \nabla f(X_{i+1}) \leq \varepsilon_i ? \]

No

Stop

\[ i = i+1 \]

Figure 3-7 Algorithm - Conjugate Gradient (Fletcher-Reeves) Method

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
problem in n variables will converge in no more than n variables. Figure 3-7 shows the algorithm for Conjugate Gradient method (Please refer Figure 6-23 and Figure 6-24 for examples of using this method).

Davidon-Fletcher-Powell Method (DFP): DFP method belongs to the family of Variable Metric Methods (VMM). It was first introduced by Davidon and several years later was developed in its current form by Fletcher and Powell. The Conjugate Gradient method’s improvement over the Steepest Descent method was possible because of the inclusion of the history from the previous iteration. In DFP method the history from all previous iterations is available. This information is collected in an \( n \times n \) matrix called the metric. The metric is updated with each iteration and is used to establish the search direction. An initial choice for the metric is also required. It must be a symmetric positive definite matrix. For the method to converge, the metric must hold on to its positive definite property through the iterations. In the DFP method, the metric approaches the inverse of the Hessian at the solution. Figure 3-8 shows the algorithm for this method (Please refer Figure 6-28 to see an example of using this method).

3.2.5.2 Constrained Optimization:

The algorithms to Constrained Optimization have two outcomes that the algorithms seek to accomplish. The first is to ensure that the design is feasible (satisfies all constraints) and the second that it is optimal (satisfies the Kuhn-Tucker conditions). Two distinct approaches will be used to handle the constrained optimization problem. The first approach is termed the indirect approach and solves the problem by transforming it into an unconstrained problem. The second approach is to handle the constraints without
transformation – the direct approach. So far, the indirect approach is implemented in TRPSEMPRO.

Choose $X_0$, $A$, $N$
\$\varepsilon_1, \varepsilon_2, \varepsilon_3$ \( \text{ (tolerance for stopping criteria) } \)
Set $i = 1$ \( \text{ (initialize iteration counter) } \)

\[ S_i = -A_i^T \nabla f(X_i) \]
\[ X_{i+1} = X_i + \alpha_i S_i; \Delta X = \alpha_i S_i \]
\( \alpha_i \) is determined by minimizing \( f(X_{i+1}) \)

\[ \nabla f(X_{i+1})^T \nabla f(X_{i+1}) \leq \varepsilon_1 \]

\( \text{YES (Converged)} \)
\[ f(X_{i+1}) - f(X_i) \leq \varepsilon_1 \]
\( \text{YES (function not changing)} \)
\[ \Delta X^T \Delta X \leq \varepsilon_1 \]
\( \text{YES (design not changing)} \)

\[ i + 1 \leq N \]
\( \text{YES (iteration limit)} \)
\[ Y = \nabla f(X_{i+1}) - \nabla f(X_i) \]
\[ Z = A_i Y \]
\[ [B] = \frac{\Delta X \Delta X^T}{\Delta X^T Y} \]
\[ [C] = \frac{ZZ^T}{Y^T Z} \]
\[ [A_{i+1}] = [A_i] + [B] + [C] \]
\[ i = i + 1 \]

Stop

Figure 3-8 Algorithm - Davidon-Fletcher-Powell Method (DFP)

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Augmented Lagrange Multiplier (ALM) method: The ALM method is the most robust of the penalty function methods. More importantly it also provides information on the Lagrange multipliers at the solution. This is achieved by not solving for the multipliers but merely updating successive SUMT (Sequential Unconstrained Minimization Techniques) iterations. Figure 3-9 shows the algorithm and Figure 6-28 shows an example of using this method.

The general optimization problem is transformed to unconstrained problem as shown in Equation (3.18) – (3.19).

Minimize:

\[ F(X, \lambda, \beta, r_h, r_g) = f(X) + r_h \sum_{k=1}^{n} h_k(X)^2 + \]

\[ \left( r_g \sum_{j=1}^{m} \max \left[ g_j(X), -\frac{\beta_j}{2r_g} \right] \right)^2 + \]

\[ + \sum_{k=1}^{n} \lambda_k h_k + \sum_{j=1}^{m} \beta_j \max \left[ g_j(X), -\frac{\beta_j}{2r_g} \right] \]  \hspace{1cm} (3.18)

Where:

\[ x^l_i \leq x_i \leq x^u_i \hspace{0.5cm} i = 1, 2, \cdots, n \] \hspace{1cm} (3.19)

Here \( \lambda \) is the multiplier vector tied to the equality constraints, \( \beta \) is the multiplier vector associated with the inequality constraints; and \( r_h \) and \( r_g \) are the penalty multipliers. \( F \) is solved as an unconstrained function for predetermined values of \( \lambda, \beta, r_h \) and \( r_g \).

Therefore, the solution for each SUMT iteration can be shown as Equation 3.20.

\[ X^* = X^*(\lambda, \beta, r_h, r_g) \] \hspace{1cm} (3.20)
Choose $X^1, N^i$ (no of SUMT iterations)
$N_m$ (no of DFP iterations)
$\varepsilon, \delta$ (for convergence and stopping)
$c^1, c^2$ (initial penalty multipliers)
$c_x, c_y$ (scaling value for multipliers)
$\lambda^1, \beta^1$ (initial multiplier vectors)
$q = 1$ (SUMT iteration counter)

Call DFP to minimize $F(X^i, \lambda^i, \beta^i, c^i, r^i)$

Output: $X^i$

If:
1. $b_i = 0$ (for $k = 1, 2, \ldots, I$)
2. $g_j \leq 0$ (for $j = 1, 2, \ldots, m$)
3. $g_j > 0$ (for $g_j = 0$)
4. all side constraints are satisfied

Then: Converged = true

Else: Converged = false

YES (Converged)

Converged = True

NO

$\Delta F = F_i - F_{i+1}, \Delta X = X^i - X^{i+1}$

YES (function not changing)

$(\Delta F)^2 \leq \epsilon^2$

NO

YES (design not changing)

$\Delta X^2 \Delta X \leq \epsilon^2$

NO

YES (maximum iterations reached)

$q = N_m$

NO

$q \leftarrow q + 1$

$\lambda^* \leftarrow \lambda^* + 2r_h(X^v)$

$\beta^* \leftarrow \beta^* + 2r_p \max(g(X^v), -\beta^*/2r_p)$

$r^*_x \leftarrow r^*_x C_x; r^*_y \leftarrow r^*_y C_y$

$X^o \leftarrow X^v$

Stop

Figure 3-9 Algorithm - Augmented Lagrange Multiplier (ALM) method

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
CHAPTER 4

SOFTWARE DESIGN FOR THE DEVELOPMENT OF
SYSTEMS ENGINEERING MODEL

Main issues about software engineering techniques and the concept of software
design patterns are introduced. Since the software tool is based on the Object-Oriented
Analysis and Design (OOA&D), detailed OO approach of designing TRPSEMPRO is
discussed. Design models are expressed by using Unified Modeling Language (UML).

4.1 Introduction to Software Engineering

4.1.1 Relationship between System Engineering
and Software Engineering

Computers are now an integral part of almost any complex system and will generally
involve software of some description which is, arguably, the most complex of man’s
creations. Software is an unpredictable beast that needs to be contained by applying
software engineering techniques that increase the chance of project success enormously.

Software engineering is a subset of system engineering that limits itself to a single
discipline. Clearly, there are many similarities between the two disciplines and it is
important to learn lessons from any source available.

40

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
4.1.2 The Phase of a Software Process

The main phases of a software process are listed in Figure 4-1 (Hans 2000). Here the Requirements analysis specifies what the application must perform, and answer the question “WHAT?”; Design specifies what the parts will be, and how they will fit together; while Implementation means code writing; and Maintenance is a continuous process for repairing defects and adding/removing components.

![Figure 4-1 Phases of Software Process](image)

This software process in Figure 4-1 is referred to as the waterfall. And it is more of an ideal or baseline than a realistic process. The spiral process, in which the waterfall is traversed several times, is commonly used in many forms. Each pass through the waterfall produces an intermediate product more capable than the previous one, until the derivable product is produced.

4.1.3 Requirements Analysis

Requirements analysis is the process of understanding, and putting in writing, a statement of what the application is intended to do once it has been built. The difficulties in creating a requirements document are: using appropriate ways to express the requirements, organizing them, and managing them over time. We express requirement in ordinary, clear, nontechnical English, from the user’s perspective; organize the requirements into logical grouping, make it easy to access and change (Jeffrey 1993).
4.1.4 Software Design

A “software design” is a set of documents on whose basis a software application can be fully programmed. In other words, a complete software design should be so explicit that a programmer could code the application from it without the need for any other documents. Software designs are like the blueprints of a building, which are sufficient for a contractor to build the required building.

The main goals of a software design are sufficiency, robustness, flexibility, reusability and efficiency (Hans 2000 and Cay 2004).

Sufficiency is the goal to satisfy the requirements for the application. Modularization is a key way to assess the sufficiency of a design: The more specific a question, the more precisely we can verify the correctness of a design that answers it; robustness makes the application to be able to handle miscellaneous and unusual conditions such as bad data, user error, programmer error, and environmental conditions; the requirements of an application can change in many ways. For example, obtaining more or less of what’s already present, adding new kinds of functionality, changing functionality and so on; flexibility is to satisfy those changing with minimum efforts of code revision.

Engineering consists of the creation of useful products with given standards of quality at minimal cost; the trend in software is to reuse parts among applications – the goal of reusability; efficiency means to create designs and implementations that are as fast as required, and which make use of no more than the available memory.

To achieve the sufficiency goal, modularizing design and reusing trusted parts need to be done; to achieve robustness goal, identification of reliable designs and robust parts is
required; to achieve reusability and flexibility goal, keeping code at a general level and minimize dependency on other class are important.

4.1.5 Design Patterns in Software Development

Experienced object-oriented developers (and other software developers) build up a repertoire of both general principles and idiomatic solutions that guide them in the creation of software. This repertoire is the design pattern – class combinations and accompanying algorithms that fulfill common design purposes. A design pattern expressed an idea rather than a fixed class combination. Accompanying algorithms express the pattern’s basic operation.

Gamma et al. (Gamma 1999) have classified each of the design patterns in one of three categories as listed follows.

- Structural patterns. Representing a collection of related objects.
- Behavioral patterns. Capturing behavior among a collection of objects.

4.2 Object-Oriented Analysis and Design (OOA&D)

OOA&D is a way of specifying and designing applications, which exploits OO technology. Its main characteristic is to approach the project under terms that occur naturally in the application. These terms are, in effect, the ingredients.

Whereas pre-OO approaches to application design and development emphasized functionality, the OOA&D approach emphasizes ingredients. In other words, “what is this application about?” The individual words (usually nouns) that answer this question
are called the domain\(^3\) classes of the application, and they appear as classes in the designs and implementation.

Usually, the use cases may not be sufficient for arriving at all of the domain classes. A brainstorming process may be required to complete the list (Cay 2004).

### OOA&D Roadmap

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Develop use case with customer</td>
<td>Determine architecture</td>
<td>Introduce design patterns or components</td>
</tr>
<tr>
<td>Convert use cases to sequence diagrams</td>
<td>Consider Framework (existing, modified, or new)</td>
<td></td>
</tr>
<tr>
<td>Seek domain classes from other sources</td>
<td>Gather domain classes Use to classify requirements</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 4-2 OOA&D Roadmap**

Figure 4-2 shows a standard way to go about effecting Object-Oriented Analysis and Design. The process realizes a major benefit of Object-Orientation. It creates a clean mapping from the very beginning between the real world, in the form of requirements,\

\(^3\) There are two kinds of classes used in designs: domain classes, which pertain to the specific application under design, and non domain classes, which are not special to this application but may be useful for this application.
and the design, in the forms of classes. The domain classes are keys in realizing this mapping.

The rest of this chapter will discuss the build of the whole application with Object-Oriented technology.

4.3 Requirement Analysis and Domain Classes Obtainment

The process to determine the domain classes is started with use cases, converting them to sequence diagrams, and selecting the classes that appear at the top of the sequence diagrams as shown in Figure 4-3.

Requirements for this project:

User can integrate any number, any kind of chemical separation models or some utility model into the whole system model as far as these models satisfy some conditions, like: they implement the defined interface, or it is some kinds simucode program which have input file, output file, executable program file.

To the user customized system model, different system analysis strategies can be applied as the user wishes.

User can view the system analysis process both in a graphical way and in a tabular way, further, user can see the result in real time.
User can specify their parameters of interest which can be viewed.

The following are key use cases for the development of a systems engineering model.

4.3.1 High Level Use Case

In the high level, there are five use cases as shown in Figure 4-4.

- System initializes the system engineering model.
- User integrates all the required models
- User builds the study plans
- User builds the solution views
- User executes the study plans which have been built.

![Sequence Diagram](image)

Figure 4-4 Use Case for System Engineering Model

According the use cases in Figure 4-4, we get the following sequence diagram to show detailed information for each use case, as shown in Figure 4-5.
4.3.2 Middle Level Use Case

Each use case in last section can be further divided into more detailed sub use cases.
4.3.2.1 Use Cases for Model Integration

Use cases for model integration include four cases as shown in Figure 4-6.

- System initializes the environment;
- User Adds/Removes models;
- User configures model properties;
- User configures parameter properties for each model, including changing values and parameter mapping.

Figure 4-6 Use Case for Model Integration

From the use cases shown in Figure 4-6, we can get the corresponding sequence diagram to show detailed information for each use case in Figure 4-6. The sequence diagram is shown in Figure 4-7.

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Figure 4-7 Sequence Diagram for ModelIntegration

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
4.3.2.2 Use case for StudyPlanBuilder:

There are four use cases for StudyPlanBuilder, as shown in Figure 4-8.

- User configures objective and constraint
- User configures study plan, study plan can be extended to two use cases, DOE study plan and optimization study plan.

![Use case diagram for StudyPlanBuilder](image)

From the use cases shown in Figure 4-8, we can get the sequence diagram for StudyPlanBuilder to show the detailed information about each use case, as shown in Figure 4-9.

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
4.3.2.3 Use case for SolutionViewer

There are five use cases for SolutionViewer as shown in Figure 4-10.

System initializes SolutionViewer

User configures graph page, including adding/removing/modifying graph page

User configures TableGraph, which can be extended to two use cases, configure graph and configure table.
From the use cases shown in Figure 4-10, we can get the corresponding sequence diagram which shows the detail information of each of use cases in SolutionViewer. Figure 4-11 shows this sequence diagram.
4.3.3 Other Issues about Obtaining Domain Class

To get the domain class, sequence diagrams are not the only sources, because some requirements do not fit within use cases; the most important source for domain classes is the set of nouns mentioned in background documents for the application.
Once candidate domain classes have been selected, they should be cut back to just the necessary ones. In fact, it is better to have too few classes at the end of this process than too many. The reason is that it’s much easier to add a class when needed than to remove a class that has become embedded in a design and implementation.

4.3.4 List of Domain Class

For the list of domain class, reader can refer to the detailed design part in section 4.5.

4.4 System Architectures

Architecture is design at a high level; we are usually more able to deal with sufficiency and flexibility than robustness and efficiency. Robustness and efficiency are usually better handled at lower levels of design.

With enough practice, it is not hard to write small programs: large applications, however, present very different problems, and are difficult to create. The principle problem of software systems is complexity – not the number of classes or lines of code per se, but their interrelationship. A very good weapon against complexity is decomposing the problem so that the result has the characteristics of small programs. For this reason, decomposing (or modularizing) the problem is of critical importance, and one of the exciting design challenges. The designer should form a clear mental model of how the application will work at a high level, and then develop a decomposition to match this mental model. This process is sometimes called recursive design because it repeats the design process at successive scales.
Effective modularization is accomplished by maximizing cohesion and minimizing coupling. This principle helps to decompose complex tasks into simpler ones. Cohesion within a module is the degree to which communication takes place among the module's elements; coupling describes the degree to which modules depend directly on other modules. Figure 4-12 shows the System Architecture for TRPSEMPro.

4.5 Detailed Design for TRPSEMPro

In this section, detailed design for TRPSEMPro is discussed. Each package shown in Figure 4-12 will be given a detailed static class diagram. The application of design pattern will be discussed here also.
4.5.1 Design for System Engineering Data Model

Figure 4-13 shows the class diagram for main data model of TRPSEMPro. In package DataModel, in order to incorporate more than one simulation program, to represent trees of object, composite design pattern are used (Robert 2003, Mark 1998). We use a recursive form to represent objects in which the tree class aggregates and inherits from the base class of the objects, TaskBase is the base class, and class ChemicalProcess, Calculation, Simcode are LeafNode which don’t aggregate other objects; class TaskProcess is NonLeafNode, and can aggregate other objects.

Client of DataModel, such as SystemManager, can reference any of the objects in the tree, and cause the object and all of its subsidiaries to perform some common actions, such as singleRun().

![Figure 4-13 Static Diagram for System Engineering Data Model](image-url)
4.5.2 Design for Modellntegration

Figure 4-15 shows the static class diagram for graph drawing in Modellntegration.

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
4.5.3 Design for StudyPlan Module

Figure 4-16 shows the static class diagram for StudyPlan Module.

![Diagram for StudyPlan Module]

4.5.4 Design for SolutionViewer Module

Figure 4-17 shows the static class diagram for SolutionViewer module.

![Diagram for SolutionViewer Module]
CHAPTER 5

AMUSE SIMULATOR AND UREX PROCESS

This chapter first introduces the design structure of AMUSE and the role of AMUSESimulator in the whole system; then, elaborates the software design about AMUSESimulator, finally, the key operations inside AMUSESimulator are overviewed.

5.1 AMUSE Code

The AMUSE (Argonne Model for Universal Solvent Extraction) code is a software package developed by Argonne National Laboratory for the analysis of a Generic UREX process which is a sub process of the whole chemical separation process as shown in Figure 1-1.

![Figure 5-1 Relationship among System Engineering Model, AMUSESimulator, and AMUSE Macro](image)

The UREX process is a solvent extraction process capable of separating small quantities of transuranic elements (for example; Np, Am, Pu, and Cm) from aqueous...
nitrate and chloride solutions. These types of chemical streams are typically generated in reprocessing plant operations or in plutonium production and purification processes.

To incorporate the AMUSE Code into the systems engineering model, AMUSESimulator program is introduced as a communication layer that allows the user to quickly and easily define the UREX process. More straightforward ways to examine different process designs will be useful for the engineering analyst.

The relationships of AMUSESimulator with systems engineering model and AMUSE macro are shown in Figure 5-1, all calculations related to uranium solvent-extraction process are made by the interaction with the MS Excel macros, defined in the ANL AMUSE codes. Also, it is not required to run AMUSESimulator with System Engineering Program TRPSEMPro together, AMUSESimulator can work with AMUSE Macro as a stand along program.

5.2 Framework of AMUSESimulator

Figure 5-2 shows the framework of AMUSESimulator. First, each of the different steps in the UREX process is outlined on the screen and allows easy modification by the user.

After all the modifications have been made, AMUSESimulator will write all the modifications into Export File which is the input file for AMUSE Macro, and triggers the execution of AMUSE Macro; at the end of AMUSE execution, a report file is generated. To expedite the data usage, AMUSESimulator provides user with the capability that all the Export File and Report File information can be saved to database – either Microsoft SQL Server 2000 database or XML database.
5.3 Design of AMUSESimulator

This section will talk about the design process for the AMUSESimulator. First, the main objects in UREX process are identified; then, according the functionality required for AMUSESimulator, the main domain classes and architecture of AMUSESimulator are obtained; finally, this section will elaborate the detailed design.
5.3.1 Objects Identification for UREX Process

Since AMUSESimulator is able to access AMUSE Macro, allow user to configure each steps in the UREX process, write this configuration to Export File, and load result from Report File, each of the processes has to be modeled to define how it is an integral part of the overall process. The process models in UREX process have been identified and the main data models in UREX process are shown in Figure 5-3.

5.3.2 Domain Class

Functions for AMUSESimulator includes (Provided by ANL):

Draw your flowsheet (sections) - we need each graphic shapes object to represent each object in UREX process.

Define your sections – we need property dialog to define sections.

Define your feed streams – we need property dialog to define streams.

Run your flowsheet – we need export file parser to read Export File and export file writer to write Export File.

View your report – we need a report file parser to read the report file, the correspondent object to store the information in Report file, and a way to display the information for that.

Summarizing from the above functionalities, the main domain classes include: Flowsheet, Section, Stream, Concentration, Stage, GFlowsheet, GSection, and GStream.

5.3.3 Architecture of AMUSESimulator

AMUSESimulator includes four main packages as shown in Figure 5-4:

SimulatorManager, IOFileParser, AMUSEDataModel, and FSGraphics.
5.3.4 Detailed Design

5.3.4.1 Detailed Design for AMUSEDataModel

AMUSEDataModel is the main package for storing and organizing all the data used in UREX process. The static diagram for AMUSEDataModel is shown in Figure 5-5.

Figure 5-5 Static Diagram for Main Data Models for AMUSESimulator
5.3.4.2 Detailed Design for FSGraphics

Figure 5-6 shows the static diagram for FSGraphics package which includes four main parts:

- FSCanvas – display Flowsheet in way of graphic blocks.
- FSStatus – display detailed flowsheet information.
- FSProperty – display the flowsheet properties list by way of table.
- FSTreeView - display the content of flowsheet by way of treeview.

![Static Diagram for FSGraphics](image)

Figure 5-6 Static Diagram for FSGraphics
5.3.4.3 Observer Design Pattern Applied to AMUSESimulator

Whenever the data source changed, all the observers must be updated. The observer design pattern, as discussed in [37] and [47], is applied here to satisfy this kind of requirements. The static diagram about the design is shown in Figure 5-7.

![Diagram of Observer Design Pattern]

Figure 5-7 Observer Design Pattern Applied to AMUSESimulator

5.4 Database Design

Database design for AMUSESimulator is shown in Figure 5-8, and XML database structure can be found in Appendix A.
Figure 5-8 Diagram for the Structure of Database Design

Figure 5-9 Dialog for Loading Flowsheet from Database
5.5 Key Operations Overview for AMUSESimulator

5.5.1 Load Flowsheet from Database

AMUSESimulator allows user to load an initial Flowsheet from either existing Export File or Database. Figure 5-9 shows the case of opening a Flowsheet from Database.

5.5.2 The Main GUI for AMUSESimulator

The main GUI for AMUSESimulator includes five parts as shown in Figure 5-10.

Menu and toolbar (Top Part) – where user can invoke all the available commands.

Flowsheet contents displayed in tree view format (Left Part) – where user can select different section, stream.

Flowsheet contents displayed in way of drawing blocks (Middle Part) – where user can select different sections, streams by clicking mouse at corresponding area.

Figure 5-10 Whole Flowsheet is Selected by Default
Property list (Right Part) – where all the properties of selected object: flowsheet, section, or stream, will be displayed and allow user to make modification.

Status Window (Lower Part) – where the detailed information of the selected object is displayed.

As shown in Figure 5-10, currently the flowsheet is the selected object, right part and down part show the information about flowsheet.

5.5.3 Property Dialog for Flowsheet

Figure 5-11 shows the property dialog for flowsheet, where the user can see and modify the properties of the flowsheet.

Figure 5-11 Property Dialog for Flowsheet
5.5.4 Select One Section.

Figure 5-12 shows the case that a section is selected; both the property window (right part) and status window (lower part) show the information about this selected section.

Figure 5-12 Section is Selected

5.5.5 Property Dialog for Section

Figure 5-13 shows the property dialog for section, where user can see and modify the properties of the selected section.
5.5.6 Select One Stream

Figure 5-14 shows the case that a stream is selected; both the property window (right part) and status window (lower part) show the information about this selected stream.
5.5.7 Property Dialog for Stream

Figure 5-15 shows the property dialog for stream, where user can see and modify the properties of the selected stream.

![Property Dialog for Stream](image)

Figure 5-15 Property Dialog for Stream

---

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
5.5.8 Utility Program: Database Viewer

Database Viewer is a utility program from which the user can look inside the database, and get all the stored run case, flowsheet, section, stream information. Figure 5-16 is a screenshot for Database Viewer.

Figure 5-16 Utility Module - Database Viewer
CHAPTER 6

CASE STUDY FOR THE DEVELOPED SYSTEMS

ENGINEERING MODEL

This chapter will give three test cases to show how the system works. Since the complex chemical separation process is still under construction in Argonne National Laboratory, here we can only give the test cases that identify the capability of the system.

6.1 Test Case 1 – Solving a Simple Optimization Problem

6.1.1 What is the Problem to Be Solved?

Minimize:

\[ f(X) = f(x_1, x_2) = 3 + (x_1 - 1.5x_2)^2 + (x_2 - 2)^2 \]  \hspace{1cm} (6.1)

Subject to:

\[ 0 \leq x_1 \leq 5; \quad 0 \leq x_2 \leq 5 \]  \hspace{1cm} (6.2)

By using TRPSEMPRo to solve this problem, we need five steps: SystemManager initialization, model integration, study plan definition, solution viewer definition, and study plan execution.

6.1.2 SystemManager Initialization

When user starts the program TRPSEMPRo, the main GUI of SystemManager is the default user interface, as shown in Figure 6-1, where user can access any other three main modules (see Figure 2-4): ModelIntegration, StudyPlan, and SolutionViewer.
6.1.3 Model Integration

When the user clicks button "ModelIntegration" in the tool bar as shown in Figure 6-1, the interface for the module, ModelIntegration, pops up as shown in Figure 6-2. By using ModelIntegration, the user can add individual models into the system engineering model. These individual models can be the calculation model, the simcode model or the chemical separation models. Figure 6-2 shows the case that a calculation model is added;

Then, the user can specify the input, output parameters for each individual model and the parameter mapping information by which the data flow among these individual models can be specified. Figure 6-3 shows parameter definition dialog, here, 2 input parameters x1 and x2, and 1 output parameter f are defined; Data flow information with parent task, TaskProcess, is also defined here.

To the calculation model, the user must add corresponding formula(s). The user can add a formula either by a graphic way as shown in Figure 6-3, or in a tabular way as
shown in Figure 6-4. After finishing the model integration, the user can go back the SystemManager interface, the newly added calculation model can be seen here, as shown in Figure 6-6; During these operations, the user can save his/her work to a XML file at any time.

Figure 6-2 Insert a Calculation Model

Figure 6-3 Define the Input and Output Parameters
Figure 6-4 Input the Formula in the Graphical Way

Figure 6-5 Input the Formula in the Tabular Way
6.1.4 Problem Definition and Study Plan Definition

After user has integrated all the individual models into our systems engineering model and specified all the data flow among each of these models, the next step would be the problem’s definition and study plan definition.

The problem’s definition includes equal and in-equal constraints definition, objective and design variables definition. As shown in Figure 6-7, we specify \( x_1 \) and \( x_2 \) to be design variable, the upper bound for both \( x_1 \) and \( x_2 \) to be 5 and lower bound to be 0; we also specify \( f \) to be the objective which will be minimized (downward arrow).

We can access the StudyPlan module by clicking the button “StudyPlan” in the toolbar as shown in Figure 6-6. Figure 6-8 shows the main interface for the StudyPlan module. From here, we can define two kinds of study plans: DOE study plan and optimization plan. Reader can reference Chapter 3 for detailed information about these techniques.
Let us first select "Design Of Experiment" in the sampling options as shown in Figure 6-8 and click the button "New". We can pop up the DOE definition dialog, as shown in Figure 6-9, where we can define the detailed information for one specific DOE study plan. Figure 6-9 shows that the specification of factors of interest, Figure 6-10 shows the specification of factors' interaction, and Figure 6-11, and Figure 6-12 shows the content of the design matrix of which each row represents the configuration of design variables for each design run.

After specifying the DOE study plan, we can specify the optimization study plan. The optimization study plan definition dialog is shown in Figure 6-12. Figure 6-13 shows the window where the user can choose the optimization technique from the four available techniques (Reference Figure 3-6, Figure 3-7, Figure 3-8 for detailed algorithms); while Figure 6-14 shows the interface where the detailed configuration for one specific optimization technique is specified.

The defined DOE study plan and optimization can be found in the main interface of StudyPlan, as shown in Figure 6-14. We can choose a single study plan or the combination of multiple study plans as the candidate study plan. In figure 6-14, the optimization study plan, "optimRandomWalk", is selected.
Figure 6-7 Problem Definition - Definition of Constraint, Objective and Design Variable

Figure 6-8 Specify Study Plan – Optimization with RandomWalk Technique
Figure 6-9 DOE Study Plan: Factor Specification

Figure 6-10 DOE Study Plan: Factor Interaction Specification
Figure 6-11 DOE Study: Design Matrix Display

Figure 6-12 Optimization Study Plan: Choose Optimization Techniques
Figure 6-13 Optimization Study Plan: Specification of Detailed Information

Figure 6-14 Add Defined Study Plan to the Calculation Model

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
6.1.5 Configure the SolutionViewer

The module SolutionViewer provides a convenient way for the user to configure how the design run result can be display. The user can access SolutionViewer by clicking button “SolutionViewer” in the toolbar shown in Figure 6-1.

The user can display the design run data in tabular form and/or chart form. Both the table and chart must be located in the graph page, as defined in TRPSEMPro. The user can add one or more graph pages, and within one graph page, one or more chart and/or table can be added.

Figure 6-15 shows the configuration dialog of graph page, user can configure how many charts and tables can be display in one specific graph page; Figure 6-16 show the chart configuration dialog. Four types of charts are provided: history chart, multi-line chart, scatter chart, and bar chart; After the chart type is selected, the parameter(s) of interest, which user want to be displayed, can be added to this chart. As shown in Figure 6-17, parameter x1, x2 and f are added to this chart. The detailed chart configuration, like position of legend, color of line, weight of line, also can be specified, as shown in Figure 6-18.

Figure 6-19 shows the table configuration dialog. Most the operations are very similar to the case of chart.
Figure 6-15 Configure Graph Page

Figure 6-16 Configuration of Chart: Select Chart Type

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Figure 6-17 Configuration of Chart: Select Parameter of Interest

Figure 6-18 Configuration of Table: Select Parameter of Interest

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
6.1.6 Execution of Study Plan

So far, individual models have been integrated, study plans have been defined, and solution viewer also has been defined. We are ready to execute the design run.

To execute the design run, we can first select the current study plan from all the defined study plans. These plans can be single run, DOE study plan, optimization study plan, or the combination of these different plan with specified execution order. In Figure 6-20, we choose the defined optimization study plan, optimRandomWalk, as the current study plan.

After choosing the current study plan, we can click the button of “Execute” in toolbar as shown in Figure 6-1.

Figure 6-21 shows the design run results displayed in both the chart and tabular way. We also can display the chart and table shown in Figure 6-21 with another separate window to get an enlarged view, as shown in Figure 6-22.

![Figure 6-19 Choose the Defined Study Plan](image-url)
Figure 6-20 Result Display: By Way of Graph Page

Figure 6-21 Result Display: In a Separate Window

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
6.1.7 Solution to this Problem

The selected start point is shown in Equation (6.3).

\[
\begin{align*}
x_1 &= 5.0 \\
x_2 &= 5.0
\end{align*}
\]  \hspace{1cm} (6.3)

The solution for this problem is shown in Equation (6.3).

\[
\begin{align*}
x_1 &= 2.99921648853126 \\
x_2 &= 1.99943718878818 \\
f &= 3.0000003204416
\end{align*}
\]  \hspace{1cm} (6.4)

6.2 Test Case 2 - Minimization of the “Banana Function”

6.2.1 The Rosenbrock function

Equation (6.5) is called the Rosenbrock function which is often used as a test problem for optimization algorithms. It is also called the banana function because of the way the

![Figure 6-22 Rosenbrock (Banana) Function](image-url)

Figure 6-22 Rosenbrock (Banana) Function

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
curvature bends around the origin as shown in Figure 6-22. It is notorious in optimization examples because of the slow convergence which most methods exhibit when trying to solve this problem.

\[ f(x_1, x_2) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2 \]  

(6.5)

6.2.2 What is the Problem: Minimization of the “Banana Function”

The problem presented here is minimization of the “Banana Function” as described in Equation (6.6) and Equation (6.7).

Minimize:

\[ f(x_1, x_2) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2 \]  

(6.6)

Subject to:

\[-2 \leq x_1 \leq 5; -2 \leq x_2 \leq 5 \]  

(6.7)

6.2.3 Solving the Problem by Using TRPSEMPro

We model this problem by way of Calculation model. The optimization techniques here adopted are both Conjugate Gradient method and RandomWalk method, and the results for those two methods are compared.

(1). Using Gradient Method: The selected start point is shown in Equation (6.8):

\[
\begin{align*}
  x_1 &= 3.0 \\
  x_2 &= 2.0
\end{align*}
\]  

(6.8)

Solution to this problem is shown in Equation 6-9. A screen shot of the solution is shown in Figure 6-23, Figure 6-24.

\[
\begin{align*}
  x_1 &= 0.879375192668678 \\
  x_2 &= 0.773655437989038 \\
  f &= 0.0145629259562806
\end{align*}
\]  

(6.9)
(2). Using RandomWalk Method: The selected start point is shown in Equation (6.10):

\[
\begin{aligned}
&x_1 = 3.0 \\
&x_2 = 2.0
\end{aligned}
\]  

(6.10)
Solution to this problem is shown in Equation 6-11. Screen shot of solution is shown in Figure 6-25, Figure 6-26.

\[
\begin{align*}
    x_1 &= 0.981806441867034 \\
    x_2 &= 0.963611644121185 \\
    f &= 0.0003420442428644
\end{align*}
\]
6.3 Test Case 3 – Application of ALM Method

6.3.1 What is the Problem to Be Solved?

Minimize:

\[ f(x_1, x_2) = x_1^4 - 2x_1^2x_2 + x_1^2 + x_1x_2^2 - 2x_1 + 4 \]  \hspace{1cm} (6.12)

Subject to:

\[
\begin{align*}
  h(x_1, x_2) : & \quad x_1^2 + x_2^2 - 2 = 0 \\
  g(x_1, x_2) : & \quad 0.25x_1^2 + 0.75x_2^2 - 1 \leq 0 \\
  0 & \leq x_1 \leq 5; \quad 0 \leq x_2 \leq 5
\end{align*}
\]  \hspace{1cm} (6.13)

6.3.2 Solving Problem by Using TRPSEMPro

Problem definition dialog is shown in Figure 6-27, \( x_1 \) and \( x_4 \) are design variables, \( f \) is the design function, \( h \) is an in-equality constraint and \( g \) is an in-equality constraint.

![Problem Definition Dialog](image)

Figure 6-27 Problem Definition Dialog
We model this problem by way of Calculation model. The optimization techniques here adopted are Augmented Lagrange Multiplier (ALM) method.

The selected start point is shown in Equation (6.14):

\[
\begin{align*}
    x_1 &= 3.0 \\
    x_2 &= 2.0
\end{align*}
\] (6.14)

The solution to this problem is shown in Equation 6.15. Screen shot of solution is shown in Figure 6-28.

\[
\begin{align*}
    x_1 &= 0.9994005161742 \\
    x_2 &= 1.00020313907996 \\
    f &= 2.99940259686877
\end{align*}
\] (6.15)

Figure 6-28 ALM Method: Solution Display in Tabular Form
6.4 Integration of Chemical Separation Process into the Developed System Engineering Model

As mentioned earlier, the complex chemical separation process is still under construction at Argonne National Laboratory; here we will just give an example to show how to integrate chemical separation process by using TRPSEMPro.

Figure 6-29 shows a flowsheet for the Glovebox phase of UREX process (see Figure 1-1 for the whole chemical separation process). We can integrate all the individual models in this flowsheet into our developed system engineering model; Figure 6-30 shows the integration result. We have already defined all the data flows between each individual models, but can not make the design run, since each of these individual blocks is still under construction.

Once all the models are implemented, we can use the way we demonstrated before, define constraint and objective, define study plan, define solution viewer, and execute the design run and do the system analysis.

Figure 6-29 Glovebox Phase of UREX Process
Figure 6-30 Integration of Chemical Separation Process:

Glovebox Phase of UREX Process
CHAPTER 7

CONCLUSION AND FUTURE RESEARCH

The whole chemical separation process, as shown in Figure 1-1, is complex to the point that definitely requires certain level of systematic coordination. To perform smoothly and meet the target extraction rates among those processes, this research proposes a general-purpose systems engineering model. Since constructing a system model is generally complex, requiring intensive communication and in-depth understanding, a carefully designed model can be more flexible and useful in the long term. This research considers design concepts from requirements definition and conceptual design to system partitioning, and finally system validation. Lengthy pre-coding of the design process and recursive modification provides a system with high degree of flexibility and robustness.

A general purposed systems engineering model, Transmutation Research Program System Engineering Model Project (TRPSEMPro), was developed based on the above design concept. The system model includes four main parts: System Manager, Model Integration, Study Plan, and Solution Viewer. System Manager supervises all the case (problem) creation, and functionality definition. Model Integration identifies chemical extraction processes and their execution sequence. Study Plan is the key to define modeling scenarios, such as Optimization, Design of Experiments, single-set parameter and multiple parameter-set. No system can be completed without a visualization tool.
Solution Viewer provides a visual means to monitor the optimization process during and after model execution. TRPSEMPro can apply not only to chemical separation process, but also a general system model, as demonstrated in chapter 6. TRPSEMPro allows industries to model their process quantitatively and to study the interactions between subsystems and performance of the model under the influence of various design parameters.

Software engineering and Object Oriented Analysis and Design (OOA&D) play a critical role during our software development. Through the application of OOA&D, we can define objects and concepts from our problem domain and is quantitatively described by Unified Modeling Language (UML). The logical software objects were created from the previous definition. Meanwhile, different design patterns were also applied during the detailed design phase. Finally, those designed components were implemented by using Microsoft®.Net, the most up-to-date object-oriented programming language framework from Microsoft.

Currently, only the UREX process module is available and ready to be implemented. Since extraction modules can be developed from various agencies with different development concepts and programming conventions, an intermediate bridge or interpreter is generally required. We are taking the only available process, UREX and linking to the TRPSEMPro system model with an interface, AMUSESimulator that communicates with the calculation engine AMUSE macros designed for UREX process. A user-friendly GUI in AMUSESimulator allows the user to efficiently define the UREX process – flowsheet, input streams, sections, and stages.
The combination of several up-to-date techniques makes this research unique and robust. Those include Microsoft.NET framework, MS SQL Server database, eXtensible Markup Language (XML), design of experiment and system optimization. The design and implementation of SQL Server Database provide an effective way to manipulate and store all the input and output data generated during the system design run. In order to analysis the system in an optimum way, several optimization technologies have been studied and correspondent algorithms have been developed and implemented in the system model. A universal XML file format is applied for data storage and transport among modules.

As pointed, UREX process is the only available separation process, and it could take years before incorporating all separation processes into the developed systems engineering model. While waiting the processes to be published, developing more system analysis modules for TRPSEMPro will definitely strengthen its capability on solving complex chemical separation process.
APPENDIX A

XML SCHEMA FOR UREX PROCESS

```xml
<?xml version="1.0" standalone="yes"?>
<xs:schema id="AmuseDataSet" xmlns=""
    xmlns:xs="http://www.w3.org/2001/XMLSchema"
    xmlns:msdata="urn:schemas-microsoft-com:xml-msdata">
  <xs:element name="AmuseDataSet" msdata:isDataSet="true">
    <xs:complexType>
      <xs:choice maxOccurs="unbounded">
        <xs:element name="tblRunCase">
          <xs:complexType>
            <xs:sequence>
              <xs:element name="case_ID">
                <xs:simpleType>
                  <xs:restriction base="xs:string">
                    <xs:maxLength value="20" />
                  </xs:restriction>
                </xs:simpleType>
              </xs:element>
              <xs:element name="gen_time" type="xs:dateTime" />
              <xs:element name="description" minOccurs="0">
                <xs:simpleType>
                  <xs:restriction base="xs:string">
                    <xs:maxLength value="500" />
                  </xs:restriction>
                </xs:simpleType>
              </xs:element>
            </xs:sequence>
          </xs:complexType>
        </xs:element>
        <xs:element name="tblFlowsheet">
          <xs:complexType>
            <xs:sequence>
              <xs:element name="case_ID">
                <xs:simpleType>
                  <xs:restriction base="xs:string">
                    <xs:maxLength value="20" />
                  </xs:restriction>
                </xs:simpleType>
              </xs:element>
              <xs:element name="gen_time" type="xs:dateTime" />
              <xs:element name="description" minOccurs="0">
                <xs:simpleType>
                  <xs:restriction base="xs:string">
                    <xs:maxLength value="500" />
                  </xs:restriction>
                </xs:simpleType>
              </xs:element>
            </xs:sequence>
          </xs:complexType>
        </xs:element>
      </xs:choice>
    </xs:complexType>
  </xs:element>
</xs:schema>
```

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
<xs:element name="FS_ID">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="20" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>

<xs:element name="Ale_suAix">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="50" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>

<xs:element name="folder_name">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="50" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>

<xs:element name="num_sections" type="xs:int" />

<xs:element name="process_temp" type="xs:double" />

<xs:element name="diluent">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="20" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>

<xs:element name="solvent_extraction_unit">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="10" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>

<xs:element name="recycle">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="10" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>

<xs:element name="TBP" type="xs:double" minOccurs="0" />

<xs:element name="CMPO" type="xs:double" minOccurs="0" />

<xs:element name="CROWN" type="xs:double" minOccurs="0" />

<xs:element name="save_DValue">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="10" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>
<xs:restriction>
    <xs:simpleType>
        <xs:element name="gen_time" type="xs:dateTime" />
    </xs:simpleType>
</xs:restriction>
<xs:element name="tblSection">
    <xs:complexType>
        <xs:sequence>
            <xs:element name="FS_ID">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="20" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="section_no" type="xs:int" />
            <xs:element name="section_name">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="20" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="num_stages" type="xs:int" />
            <xs:element name="frac_efficiency" type="xs:double" />
            <xs:element name="QFAI" type="xs:double" minOccurs="0" />
            <xs:element name="aq_feed_cl" minOccurs="0">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="1" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="QFOI" type="xs:double" minOccurs="0" />
            <xs:element name="org_feed_cl" minOccurs="0">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="1" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="FEAI_input" type="xs:double" minOccurs="0" />
            <xs:element name="aq_eff_cl" minOccurs="0">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="1" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="FS_ID">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="20" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="section_no" type="xs:int" />
            <xs:element name="section_name">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="20" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="num_stages" type="xs:int" />
            <xs:element name="frac_efficiency" type="xs:double" />
            <xs:element name="QFAI" type="xs:double" minOccurs="0" />
            <xs:element name="aq_feed_cl" minOccurs="0">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="1" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="QFOI" type="xs:double" minOccurs="0" />
            <xs:element name="org_feed_cl" minOccurs="0">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="1" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="FEAI_input" type="xs:double" minOccurs="0" />
            <xs:element name="aq_eff_cl" minOccurs="0">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:maxLength value="1" />
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
</xs:element>
<xs:element name="FEIO_input" type="xs:double" minOccurs="0" />
<xs:element name="org_eff_cl" minOccurs="0">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="1" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>
<xs:element name="reroute_aq_sec" minOccurs="0">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="2" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>
<xs:element name="reroute_org_sec" minOccurs="0">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="2" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>
<xs:element name="FAI_input" type="xs:double" minOccurs="0" />
<xs:element name="FOI_input" type="xs:double" minOccurs="0" />
<xs:element name="section_cl">
  <xs:simpleType>
    <xs:restriction base="xs:string">
      <xs:maxLength value="1" />
    </xs:restriction>
  </xs:simpleType>
</xs:element>
</xs:sequence>
</xs:complexType>
<xs:element name="tblStage">
  <xs:complexType>
    <xs:sequence>
      <xs:element name="FS_ID">
        <xs:simpleType>
          <xs:restriction base="xs:string">
            <xs:maxLength value="20" />
          </xs:restriction>
        </xs:simpleType>
      </xs:element>
      <xs:element name="section_no" type="xs:int" />
      <xs:element name="stage_no">
        <xs:simpleType>
          <xs:restriction base="xs:string">
            <xs:maxLength value="10" />
          </xs:restriction>
        </xs:simpleType>
      </xs:element>
    </xs:sequence>
  </xs:complexType>
</xs:element>

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
</xs:unique>
<xs:unique name="tblFlowsheet_Constraint1" msdata:ConstraintName="Constraint1"
msdata:PrimaryKey="true">
  <xs:selector xpath="./tblFlowsheet" />
  <xs:field xpath="FS_ID" />
</xs:unique>
<xs:unique name="tblSection_Constraint1" msdata:ConstraintName="Constraint1"
msdata:PrimaryKey="true">
  <xs:selector xpath="./tblSection" />
  <xs:field xpath="FS_ID" />
  <xs:field xpath="section_no" />
</xs:unique>
<xs:unique name="tblStage_Constraint1" msdata:ConstraintName="Constraint1"
msdata:PrimaryKey="true">
  <xs:selector xpath="./tblStage" />
  <xs:field xpath="FS_ID" />
  <xs:field xpath="section_no" />
  <xs:field xpath="stage_no" />
</xs:unique>
</xs:element>
</xs:schema>
APPENDIX B

XML SYSTEM ENGINEERING MODEL DESCRIPTION FILE

<?xml version='1.0'?>
<schema xmlns="http://www.unlv.edu/ncacm/TRPSEMPro/XMLSchema">
<! Task XML File - Author: Lijian Sun-->
<Task Name="TaskProcess" Type="TASK_PROCESS">
<ParameterList>
<Parameter Name="x1" Category="input" Type="real">
  <Initial Value>0</Initial Value>
  <Var Indicator>POTENTIAL_DESIGN_VAR</Var Indicator>
  <Obj Indicator>POTENTIAL_OBJ</Obj Indicator>
  <Cur Value>0</Cur Value>
  <Lower Bound Value>0</Lower Bound Value>
  <Upper Bound Indicator>No_LBound</Upper Bound Indicator>
  <Upper Bound Value>0</Upper Bound Value>
  <Description>
  </Description>
</Parameter>
</ParameterList>
<Parameter Name="f" Category="output" Type="real">
  <Initial Value>0</Initial Value>
  <Var Indicator>POTENTIAL_DESIGN_VAR</Var Indicator>
  <Obj Indicator>POTENTIAL_OBJ</Obj Indicator>
  <Cur Value>0</Cur Value>
  <Lower Bound Value>0</Lower Bound Value>
  <Upper Bound Indicator>No_LBound</Upper Bound Indicator>
  <Upper Bound Value>0</Upper Bound Value>
  <Description>
  </Description>
</Parameter>
<Parameter Name="x2" Category="input" Type="real">
  <Initial Value>0</Initial Value>
  <Var Indicator>POTENTIAL_DESIGN_VAR</Var Indicator>
  <Obj Indicator>POTENTIAL_OBJ</Obj Indicator>
  <Cur Value>0</Cur Value>
  <Lower Bound Value>0</Lower Bound Value>
  <Upper Bound Indicator>No_LBound</Upper Bound Indicator>
  <Upper Bound Value>0</Upper Bound Value>
</Parameter>
</Task>
</schema>
<DataFlow>from_to</DataFlow>
</MapInformation>
</Parameter>
</ParameterList>
</TaskPlansTemplate>
<Plan Name="optimRandomWalk" Category="Optimization">
<OptimTechList>
<OptimTech>
<Type>RandomWalk</Type>
<NumIterations>50</NumIterations>
<Tolerance>0.0001</Tolerance>
<InitValueStepSize>0</InitValueStepSize>
<IncrementalValue>1</IncrementalValue>
<NumScanSteps>20</NumScanSteps>
</OptimTech>
</OptimTechList>
</Plan>
<Plan Name="Optim_ConjugateGradient" Category="Optimization">
<OptimTechList>
<OptimTech>
<Type>ConjugateGradient</Type>
<NumIterations>30</NumIterations>
<Tolerance>0.0001</Tolerance>
<InitValueStepSize>0</InitValueStepSize>
<IncrementalValue>1</IncrementalValue>
<NumScanSteps>20</NumScanSteps>
</OptimTech>
</OptimTechList>
</Plan>
<Plan Name="Optim_DFP" Category="Optimization">
<OptimTechList>
<OptimTech>
<Type>DFP</Type>
<NumIterations>30</NumIterations>
<Tolerance>0.0001</Tolerance>
<InitValueStepSize>0</InitValueStepSize>
<IncrementalValue>1</IncrementalValue>
<NumScanSteps>20</NumScanSteps>
</OptimTech>
</OptimTechList>
</Plan>
<Plan Name="DOEStudy" Category="DOEStudy">
<ParameterDOEList>
<ParameterDOE>
>Name=x1</Name>
<Category>input</Category>
<IsFactor>True</IsFactor>
<LevelTypeIndicator>%</LevelTypeIndicator>
<Values>-25 25</Values>
<BaseLine>0</BaseLine>
</ParameterDOE>
</ParameterDOEList>
</DOEStudy>
<ParameterDOE>
  <Name>f</Name>
  <Category>output</Category>
  <IsFactor>False</IsFactor>
  <LevelTypeIndicator>%</LevelTypeIndicator>
  <Values>-25 25</Values>
  <BaseLine>0</BaseLine>
</ParameterDOE>

<ParameterDOE>
  <Name>x2</Name>
  <Category>input</Category>
  <IsFactor>True</IsFactor>
  <LevelTypeIndicator>%</LevelTypeIndicator>
  <Values>-25 25</Values>
  <BaseLine>0</BaseLine>
</ParameterDOE>

<ParameterDOEList>
</ParameterDOEList>

<Plan>
</Plan>

<TaskPlansTemplate>
<TaskPlans>
  <Plan Name="optimRandomWalk" Category="Optimization">
    <OptimTechList>
      <OptimTech>
        <Type>RandomWalk</Type>
        <NumIterations>50</NumIterations>
        <Tolerance>0.0001</Tolerance>
        <InitValueStepSize>0</InitValueStepSize>
        <IncrementalValue>1</IncrementalValue>
        <NumScanSteps>20</NumScanSteps>
      </OptimTech>
    </OptimTechList>
  </Plan>
</TaskPlans>

<FormulaList>
  <Formula>f = 3+ ( x1-1.5*x2 ) ^2 + (x2-2)^2</Formula>
</FormulaList>
</Task>
</Task>

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
BIBLIOGRAPHY


Gamma E., R. Helm, R. Johnson, and J. Vlissides, Design Patterns: Elements of Reusable Object Oriented Software, Addison-Wesley, 1999.


Deitel, Deitel, Listfield, Nieto, Yaeger, Zlatkina, C# how to program, Prentice Hall, 2002.

Tomasz Mdlner, C++ Programming with Design Patterns Revealed, Addison Wesley, 2002.


Michael J. Laszlo, Object-Oriented Programming Featuring Graphical Applications in Java, Addison-Wesley, 2002.


R. Allen Wyke, Sultan Rehman, Bradley Leupen, XML Programming (Core Reference), Microsoft Press, c2002.


The XML industry portal. XML.ORG, URL: http://www.xml.org/xml/resources_cover.shtml (viewed 2003)


VITA

Graduate College
University of Nevada, Las Vegas

Lijian Sun

Local Address:
1600 E. University Ave #231
Las Vegas, NV, 89119

Degrees:
Bachelor of Science, Mechanical, 1995
Hebei University of Technology, Tianjin, P.R.China

Master of Science, Mechanical, 2001
Hebei University of Technology, Tianjin, P.R.China

Publications:
“Reverse Engineering of Free Surface to Rapid Prototype and Software Realization”,

Lijian Sun, Anping Xu, Runhua Tan, The Application of Reverse Engineering in
Rapid Prototype Manufacture, Journal of Hebei University of Technology, Vol. 28
No.6, December 1999, p22-27.

Lijian Sun, Yitung Chen, Randy Clarksean, Darrell Pepper, Development of a
Systems Engineering Model of the Chemical Separations Process, American Nuclear
Society Conference, Hilton Resort & Casino, Reno, Nevada, USA, November 10-11,

Lijian Sun, Jianhong Li, Yitung Chen, Randy Clarksean, Darrell Pepper,
Development of a Systems Engineering Model of the Chemical Separations Process,
International Congress on Advanced Nuclear Power Plants in Hollywood, Florida,

Lijian Sun, Steven Lei, Yitung Chen, Hsuan-Tsung Hsieh and Darrel Pepper,
Environmental Data Management System - From Data Monitoring, Acquisition,
Presentation to Analysis, 15th International Conference on Parallel and Distributed

Lijian Sun, Steven Lei, Yitung Chen, Hsuan-Tsung Hsieh, Darrel Pepper, Data Acquisition and Monitoring System - A State Funded Air Quality Monitoring System Development, 15th International Conference on Computer Applications in Industry and Engineering, Clarion Hotel Bay View, San Diego, California, USA, November 7-9, 2002.


Thesis Title:
Development of a Systems Engineering Model for the Chemical Separation Process

Thesis Examination Committee:
Chairperson, Dr. Yitung Chen, Ph. D.
Committee Member, Dr. Robert F. Boehm, Ph. D.
Committee Member, Dr. Hsuan-Tsung (Sean) Hsieh, Ph. D.
Graduate Faculty Representative, Dr. Yahia Baghzouz, Ph. D.