Chapter I

INTRODUCTION

1.1 Motivation

Chemical process converts the raw material into the needful products. Now a day, optimization tools are widely employed to get the desired process efficiency in chemical process. This demands, optimization of the model based analysis of existing process plant to improve the operating variable and conditions which may affect the environment in order to reduce the investment cost and operating cost. In this context, however, one of the remarkable aspects of science is it ability to rigorously characterize the relative strength of the inferences and communicate the level of uncertainty associated with certain types of claims. That is, the degree of uncertainty can be graded, which surround certain scientific claims so that their strengths can be widely understood and compared.

1.2 Optimization in Chemical Industries

The optimization of the process plant has many possible objectives such as to maximize the production, product value or profit and to minimize operating costs or to minimize the wastes. The role of optimization is to evaluate the values of process variables subject to the conditions and constraints, so that there is always an improvement in the overall economics of the process plant. Determination of the optimum conditions or variables in process industries consists of two widely separated steps. The first step is the formulation of the design optimization problem. The second step is the determination of solution to the chosen optimization problem.
1.3 Classical Search and Optimization Methods

Traditional optimization methods used for design can be classified into two distinct groups: i) Direct search method and ii) Gradient-based methods. In direct search methods, objective function and constraint values are used to guide the search strategy. Gradient based methods use the first or second-order derivatives of the objective function and constraints to guide the search process.

Direct search methods are usually slow, requiring many evaluations for convergence, as derivative information is not used by these techniques. Gradient-based methods quickly converge to an optimal solution, but are not efficient in problems where the function is non-differentiable or discontinuous in nature (Reklaitis et al., 1983). Every traditional optimization technique is designed to solve a specific type of problem. For example, the geometric programming method is designed to solve polynomial type objective functions. They cannot be applied suitably to solve other types of functions. The conjugate direction or conjugate gradient methods have convergence proof for solving quadratic objective functions having one optimal solution but are not expected to work well in problems having many solutions (Rao, 1996).

Frank-Wolfe successive linear programming method works efficiently on linear functions, but for solving nonlinear problems its performance largely depends on the chosen initial conditions. Thus one technique may be best suited for a particular type of problem and may not even be applicable to solve a different problem. This demands the engineers to know a number of optimization algorithms to solve the design problems.

To overcome the drawbacks of the conventional optimization techniques, this thesis aims to employ a single optimization technique namely genetic algorithm and
differential evolution algorithm which is able to solve all the optimal design problems in the area of process engineering.

1.4 Evolutionary Algorithms

There has been an increasing interest recently in the use of evolutionary optimization techniques to solve the scheduling problems. Evolutionary computation based search algorithms like Genetic Algorithm (GA), Evolutionary Strategy (ES), Evolutionary Programming (EP), Genetic Programming (GP) and Differential Evolution (DE) are very efficiently in solving highly nonlinear problems.

An evolutionary computation approach begins by initializing a population of candidate solutions to a problem. New solutions are then created by randomly varying those of the initial population. All solutions are measured with respect to how well they address the problem. Finally, a selection criterion is applied to arrange out those solutions that are below similarity. The process is continued using the selected set of solutions until a specific criterion is met. The advantages of evolutionary computation are its adaptability to change and ability to generate good enough solutions.

1.4.1 Genetic Algorithm

Darwin’s Theory of Evolution states that all life is related and has descended from a common ancestor. The theory presumes that complex creatures have evolved from more simplistic ancestors naturally over time. In a nutshell, as random genetic mutations occur within an organism's genetic code, the beneficial mutations are preserved because they aid survival -- a process known as "natural selection." These beneficial mutations are passed on to the next generation. Over time, beneficial mutations accumulate and the result is an entirely different organism.
Genetic algorithms are adaptive heuristic search algorithm premised on the Darwin’s evolutionary ideas of natural selection and genetics. The basic concept of GA are designed to simulate processes in natural system necessary for evolution. As such they represent an intelligent exploitation of a random search within a defined search space to solve a problem. First pioneered by John Holland in the 60’s, GAs has been widely studied, experimented and applied in many fields in engineering world. Not only does genetic algorithm provide an alternative method to solving problem, it consistently outperforms other traditional methods in most of the problems link. Many of the real world problems which involve finding optimal parameters might prove difficult for traditional methods but are ideal for genetic algorithms.

1.4.2 Differential Evolution Algorithm

Differential Evolution (DE) is a numerical optimization approach developed by Storn and Price (1997). DE is simple, easy to implement, significantly faster and robust. The fittest offspring competes one-to-one with its parent, which is different from the other evolutionary algorithms.

Differential Evolution has been verified as a promising candidate for solving real-valued engineering optimization problems. The present work is concerned with the development of efficient method for chemical process plants based on differential evolution and its variants. The emphasis has been mainly to develop simpler and flexible models that can effectively handle the operating parameters and result in schedules that are cost effective and acceptable in operation and in computation. Figure 1 shows the structure of the DE algorithm.
Optimization of Chemical Process Plant using Evolutionary Algorithms

Figure 1.1 Flow chart of DE algorithm

The differential evolution based approach is a single candidate for solving different operating variables of process plants. Thereby, the need for other optimization techniques does not arise. Thus, this thesis concerns a search for the feasibility and efficiency of differential evolution in solving the chemical process plant problem. The aim of this thesis is to take the advantage of strengths of differential evolution and employing strategies for making it more suitable for the needs of the chemical process plants.
1.5 Optimization under Uncertainty

The uncertainty associated with a piece of scientific knowledge provides a measure of its practical epistemological robustness. It represents the degree to which our knowledge concerning the relevant physical phenomenon is imperfect. Although uncertainty may be minimized, it cannot be eliminated: it is inherent to all scientific knowledge. Science has developed methods for rigorously characterizing and communicating the level of uncertainty associated with certain types of claims. The X bar and S control chart, indicate whether the sample data fall within the upper and lower control limit. The process capability test permits the uses to assign a “degree of belief” that can be placed in such knowledge expressed as a likelihood or level of confidence.

1.6 Optimal Design of Process Plant

Chemical industries have undergone significant changes due to increase in the cost of energy and stringent environmental regulations. Modifications in plant design procedures and in operating conditions have been implemented in order to reduce the cost. Chemical reactors are usually the central point in a process industry and their function frequently determines the economics of the entire process. The operation of reactor has a direct effect on raw material cost as the design and operation, wanting in optimization, may overcome the wastage of raw materials. The composition of reactor outlet stream determines the size and hence the cost of the downstream units associated with the reactor. Therefore, it is evident that the optimum operating conditions for a chemical process are closely associated with the design and operation of the reactor.
1.7 Novelty

Present need of the engineering community aims at cost minimization both fixed and operating cost, which accounts for technical, economical, environmental and safety criteria of the chemical process plant.

- The paradigm shift in technical know-how leads to enhanced yield and quality of the product demands. It is addressed in this work by optimizing the design, operation and design variables of the chemical process plants.

- The economics of the process exploits the advantage of rate of production, lower energy consumption, reduction in material and improved efficiency of continuous process. The cost reduction can be passed on to the consumer thus benefitting the society without compromising the profit. This is adequately addressed by, reducing the annual cost by using the cost objective function of the chemical process plant.

- The environmental and the safety criteria calls for the operation to be inherently safety and environmental friendly, hence making it compliant with the existing norms and regulations of the government and other statutory agencies. Making the process safe results in curtailing direct and indirect costs associated with the non compliance of norms and other hazards. This study takes into consideration uncertainty of the control variables to make it as robust addressed by tolerance limits.
1.7.1 Scope of the Study

Based on these ideas and the immense literature information in background, the objectives of the present investigations are:

- **Development and implementation of Differential Evolution (DE) algorithm for Reactor and Heat Exchanger (RHE) system, Williams Otto Process Plant (WOPP) and Multiproduct Industrial Process Plant (MIPP).**

- **Performance analysis of these algorithms in terms of**
  - Minimizing the volume of reactor and reducing capital cost at RHE.
  - Maximizing the percentage returns on investment and minimize the volume of the reactor at WOPP.
  - Minimizing the capital cost, volume of the reactor and batch size and the cycle time of products at MIPP.

- **The comparison of the outcomes made with Differential Evolution (DE) and Genetic Algorithm (GA).**

- **Testing of Process Capability for Uncertainty**
  - In all the above mentioned three chemical process plants, the process variables have inherent limitations on how narrowly it can characterize the value of a quantity of interest.
  - In order to account for those limitations, the X bar and S control chat is used to verify whether the sample data are within control.
  - Then carried out process capability test using the normal distribution and fix the tolerance limits for the control variable to minimize the uncertainty.
The dissertation is organized as follows:

- **An insight into the organization of the work carried out in this research is presented in Chapter 1.**

- **Chapter 2** covers the brief review of the literature on Genetic Algorithm (GA), Differential Evolution (DE) algorithm, Reactor and Heat Exchanger system (RHE), Williams Otto Process Plant (WOPP), Multiproduct Industrial Process Plant (MIPP) and optimization under uncertainties.

- Descriptions of Genetic Algorithm (GA), Differential Evolution (DE) algorithm, optimization under uncertainty are furnished in Chapter 3.

- General Mathematical Modelling, Mathematical Modelling with objective function for the three chemical processes such as Reactor and Heat Exchanger system (RHE), Williams Otto Process Plant (WOPP), Multiproduct Industrial Process Plant (MIPP) are presented in Chapter 4.

- **Chapter 5** deals in detail on the results and discussion.

- The conclusion of the dissertation, highlighting the contribution of this research work to the field knowledge is provided in Chapter 6.