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## The Basic Ideas

### 1.1 Introduction

A typical industrial process passes through many stages of development. Thus, in the evolution of a chemical process to produce a certain product, first comes the idea for a promising manufacturing step, followed by long laboratory work to approve concept. The laboratory results provide a preliminary estimate of feasibility and may lead to the possible industrial process. Those results may then be used to build a pilot plant. The pilot plant is a next step between lab and full scale and will have sufficient flexibility to test more extreme conditions. Engineers will use data from pilot plant to design a full-scale plant. Assuming that the plant is built then, ideally, plant will run with operating conditions generated from lab and pilot plant. The small-scale work will have provided estimates of process parameters like concentrations, temperatures, pressures, and flow rates. These estimates of process conditions represent only good first guesses in a continuing process adjustment. This is the reason for special attention to plant startup. A special technical team is usually assigned during the startup, since it is realized that major adjustments may be necessary before the process can be made to perform reasonably well (or sometimes to perform at all).

With startup phase completed, a further stage of iteration has been gone through and, hopefully, the process will produce a stable product. The most likely is that product is being produced at lower production rate, at lower yield, and at lower quality than the plant is capable of. The process of “fine tuning” still remains to be done. This “tuning” or optimization process is the main subject of this book.

It is common to find chemical process 10 years after startup with production rates two or three times those originally thought possible, with major yield increases, and with a product of greatly improved quality [1]. Before optimization can be conducted, precise representations of the process, or models, have to be built.

There are two methods, available for chemical engineer, to build a model:

- DM – Data mining, using Historical Data (Data Historian) and neural network modeling technique to build model.
- DOE – Design of experiment to build a regression model based on experimental data.

Whenever feasible, the alternative of taking new data to build a model is preferable. This approach is supported by long practical experience. A rule of thumb is that an experimental design – DOE, executed according to the principles, has a 90% or better chance of obtaining the information required for meeting the objective.

An analysis of historical data typically has only a 10–20% chance of success, even though hundreds/thousands of data points may be available.

Typical defects in historical data are:

- The independent variables-factors are often highly confounded, making determination of their effects difficult and ambiguous.
- Independent variables will often vary over narrow ranges, since the process has been operating with the intention of making uniform product, not for the purpose of demonstrating the effects of the factors.
- The lack of the randomization leads to large bias errors.
- The data often contain many erroneous bad data that must be corrected or deleted before further analysis.
- Proportion of data where one or more variables have missing data is often large. One missing factor disqualifies an entire row in regression analysis.

Historical Databases–Data Historians are more widely available with the proliferation of on-line process computers and database management programs. In many cases, the abundance of numbers greatly exceeds the useful information contained in the data.

Frequently, more than half of the effort in the analysis of historical data is required to clean up the files to a state that will yield preliminary estimates of descriptive statistics. Furthermore, the successful analysis of historical data requires the skills of a statistician experienced in the analysis of “messy data.” The latest breakthrough in process modeling and optimization is based on historical data and neural network with fuzzy logic is used for nonlinear modeling. The “Process Insights”<sup>1</sup> (Pavilion Technologies Co.) is one of the best neural network model-based applications for chemical industry.

These remarks should not be accepted as a reason against all analyses of historical data. Such analyses are necessary in fields of economics and social science, where direct experimentation is difficult if not impossible. But in the fields of engineering and technology, where direct experimentation is possible, the chances of success are greatly enhanced by using the DOE strategy [3]. As a preliminary step for designed experimentation, simple plotting of historical data is often useful to obtain a clue for potential problem cause and suggestion for the next steps. On the other hand, the design, execution, and analysis of well-planned experiment will often be less costly in both time and money than an elaborate and massive analysis of historical data. The special DOE software packages available are “Design Expert,”<sup>2</sup> “Echip,”<sup>3</sup> “MiniTab,”<sup>4</sup> etc.

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1 Process Insights, Pavilion Technologies Co., Austin, TX, USA.

2 Design-Expert, Stat-Ease, Inc., Minneapolis, MN, USA.

3 ECHIP, Incorporated, 724 Yorklyn Road, Hockessin, DE, USA.

4 Minitab LLC, State College, Pennsylvania, USA.