CHAPTER
1

Chapter 1. Introduction

1.1 Importance of Process Control

Process control is one of the foremost necessities in any processing plant. Design of efficient control system is essential for (Stephanopoulos, 1984), (LeBlanc & Coughanowr, 2013) :

a) Ensuring safety of the plant operators and others,

b) Maintaining various operating variables (concentration, pressure, temperature, etc.) at the desired levels to ensure safety of the plant equipment,

c) Achieving desired levels of product quality and quantity for improved marketability,

d) Insuring energy efficiency,

e) Optimum consumption of raw materials,

f) Maintaining the desired discharge levels of various pollutants into the land/air/water bodies as per the norms prescribed by the enforcing agencies, and

g) Monitoring and diagnosis of plant equipment health (Marlin, 1995).

1.2 Challenges in Controller Design

Design and implementation of efficient control systems for chemical processes is a challenging task due to:

a) Process nonlinearity,

b) Steady state multiplicity (Bequette, 1998),

c) Process instability (Right Half Plane (RHP) pole, dead time),

d) Minimum/non-minimum phase behaviour (RHP/Transmission zeros) (Bequette, 2003),

e) Time varying process parameters,

f) Control loop interactions (Multivariable control),

g) Process uncertainty (poor knowledge of the complete process),

h) External disturbances/interferences, and

i) Lack of robustness

1.3 Importance of Process Modeling and Identification in Control

The foremost requirement for the design of an efficient control system for any process /plant is to have a thorough and complete understanding of its static (steady state) and dynamic (transient) behaviour. Modeling of the process is therefore very crucial for designing a control system design since it provides qualitative and quantitative information about the input-output functionality required for the process.

In most cases, it is highly convenient to represent the actual physical process in terms of an appropriate mathematical analogue, known as the process model. The process of the development of a truly representative process model is referred to as 'Modeling'. Mathematical models are obtained by applying various conservation laws (unsteady state total mass balances, component balances, energy balances, momentum balances), Thermodynamic equations of state, chemical and phase equilibrium relationships, reaction kinetics etc. as applicable to a process (Jensen et al., 1977), (Loney, 2006).

The process may also be well studied at a molecular/microscopic/macroscopic level, depending upon the required depth and rigor of the analysis. Process modeling, at the end of the day, results in a set of mathematical equations (differential/algebraic) in terms of the process variables and system's parameters.

Identification, on the other hand, is the process of developing mathematical models using a vast and diverse range of experimental data to build empirical correlations among the different input-output process variables and parameters, in the absence of clear/complete understanding of the underlying scientific phenomena (Ogunnaike, 2020) (Sánchez et al., 2012).

Examples of process identification in chemical engineering include empirical correlations for obtaining the heat transfer coefficients (Nusselt number) under turbulent flow conditions, based on experimental data Reynolds number and Prandtl number. In the area of process control, identification refers to the activity of estimating the process parameters (gain, time constant etc.) of transfer function models to be used as an integral part in the design of control systems (Liu & Gao, 2011) (Ikonen & Najim, 2001), (Englezos & Kalogerakis, 2000)

1.3.1 Desirable Characteristics of Process Model

Process models are selected on the basis of one or more of the following desirable characteristics:

a) Sensitivity

Input sensitivity/Parametric sensitivity is the measure of change in model output with respect to change in the process input variable or parameter

b) Accuracy

Accuracy is the measure of the 'goodness of fit'. It is quantified as the minimum deviation of model output (prediction) from the desired value.

c) Generalization capability

Generalization capability refers to the ability of the model to provide accurate predictions over a wide range of changes in input conditions or process parameters

d) Flexibility

Flexibility of process model is its capability to provide the best fit covering/encompassing a wide range of data points (Pitt et al., 2008). Model flexibility is improved by incorporating higher number of parameters in the regression space or by increasing the polynomial order as the case may be. Even though, an increase in the model flexibility improves the model accuracy, it comes at the cost of generalization capability. A trade-off between model flexibility and generalization capability is therefore required to be achieved.

1.3.2 Classification of Process Models

Process models are classified as theoretical, empirical, black-box, grey-box, lumped parameter, distributed parameter, space-state, and Laplace transform models.

a) Theoretical (First Principles based) (White-box) Models

The Theoretical models are developed based on the first principles when a complete insight of the process is available (Varma et al., 1997); (Roffel & Betlem, 2007); (Corriou, 2010). The advantages of such models are high accuracy and generalization capability. However, the theoretical models being highly complex are cumbersome and involve huge processing time and memory cost. Theoretical models may also lack sensitivity when the processes have time varying parameters.

b) Empirical (correlation based) Models

The empirical models, often used in process identification, are based on correlations among the process variables. They are used when the physics of the process is not completely understood. They are based on fitting experimental data to a selected functional relation between the input and output. Linear or nonlinear parameter estimation techniques are used to obtain the optimum values of model parameters. The functional relation between the input and output is often selected on the basis of a definite scientific understanding of the process.

c) Data driven (Black-box) Models

Data driven black box models are used when no proper insight of the process is available but a large set of input-output experimental/plant data is available. These models involve selecting a complex multi-layered network of mathematical functions called activation functions. The parameters involved in the network of activation functions (known as weights, biases etc.) are optimized using a suitable nonlinear optimization algorithm (Example: The Levenberg-Marquardt method) The most common examples of data driven black box models are the Artificial Neural Network (ANN) , Fuzzy logic and Wavelet based models. In order to train the models, the available input-output experimental/plant data is initially segregated into- (a) Training data set, and (b) Prediction/Test data set. The model (Network) parameters are optimized by training the model on the training data set and evaluating its performance on the test data set based on the quantitative performance indices (QPIs) such as Sum of Squares of Errors (SSE), Correlation coefficient etc. Purely data driven models permit higher sensitivity and accuracy but lack generalization capability. For example: ANN models are known to work well on 'seen' data. ANN models on the other hand have the reputation of being bad extrapolators.

d) Hybrid (Grey-box) Models

Hybrid (Grey-box) models combine the capabilities of both theoretical and black box models.

e) Lumped parameter/capacity models

In lumped parameter/capacity models, only the time variation of variables is considered whereas the spatial variation is neglected, (Luyben, 1990), (Franks & Franks, 1972) . Example, in a Continuous Stirred Tank Reactor, if the assumption of perfect mixing is valid, the spatial variation of concentration and Temperature are neglected and under unsteady state conditions, only the time variation is of interest. Since these models involve only one independent variable (time), the resulting mathematical model comprises of a set of Ordinary differential equations (ODEs) and are often solved as ODE IVPs (Initial value problems).

f) Distributed parameter models

Distributed parameter models involve both time and spatial variation of variables. For example, in plug flow reactors (PFRs) and heat exchangers, the study of variation of concentration and/or Temperature along the length of reactor/heat exchanger as well as the time variation of process variables at any fixed location is equally important (Harriott, 1984). Since the distributed parameter models involve more than one independent variable (space and time), the resulting mathematical model comprises of a set of Partial differential equations (PDEs) and are often solved making use of appropriate boundary conditions (PUSHPAVANAM, 1998) , (Rice & Do, 2012).

g) State space models (time domain)

State space models are (linearized) dynamic models that represent the mathematical relationships (differential equations) among the states of the system (referred to as the state variables) and the input variables (Lipták, 2018). The state space models are very useful in obtaining essential quantitative information on (a) the steady state solution, (b) perturbation, speed of response and stability (based on Eigen values and Eigen vectors, and (c) dynamic response of the process to an input sequence

h) Transfer function models (Laplace domain)

Transfer function models are very useful in the process control arena for studying the open loop and closed loop behaviour of process. Transfer function models are directly obtained from the (linearized) state space models of the process, by taking Laplace transform. Transfer function models represent the ratio of change in output variable (controlled variable) to change in the input variable (Manipulated or Disturbance variable) Chemical processes mostly involve multiple variables and hence require more than one transfer functions (Transfer function matrix) for control system design.

The importance of process modeling and identification in the area of control is depicted in Figure 1.1.

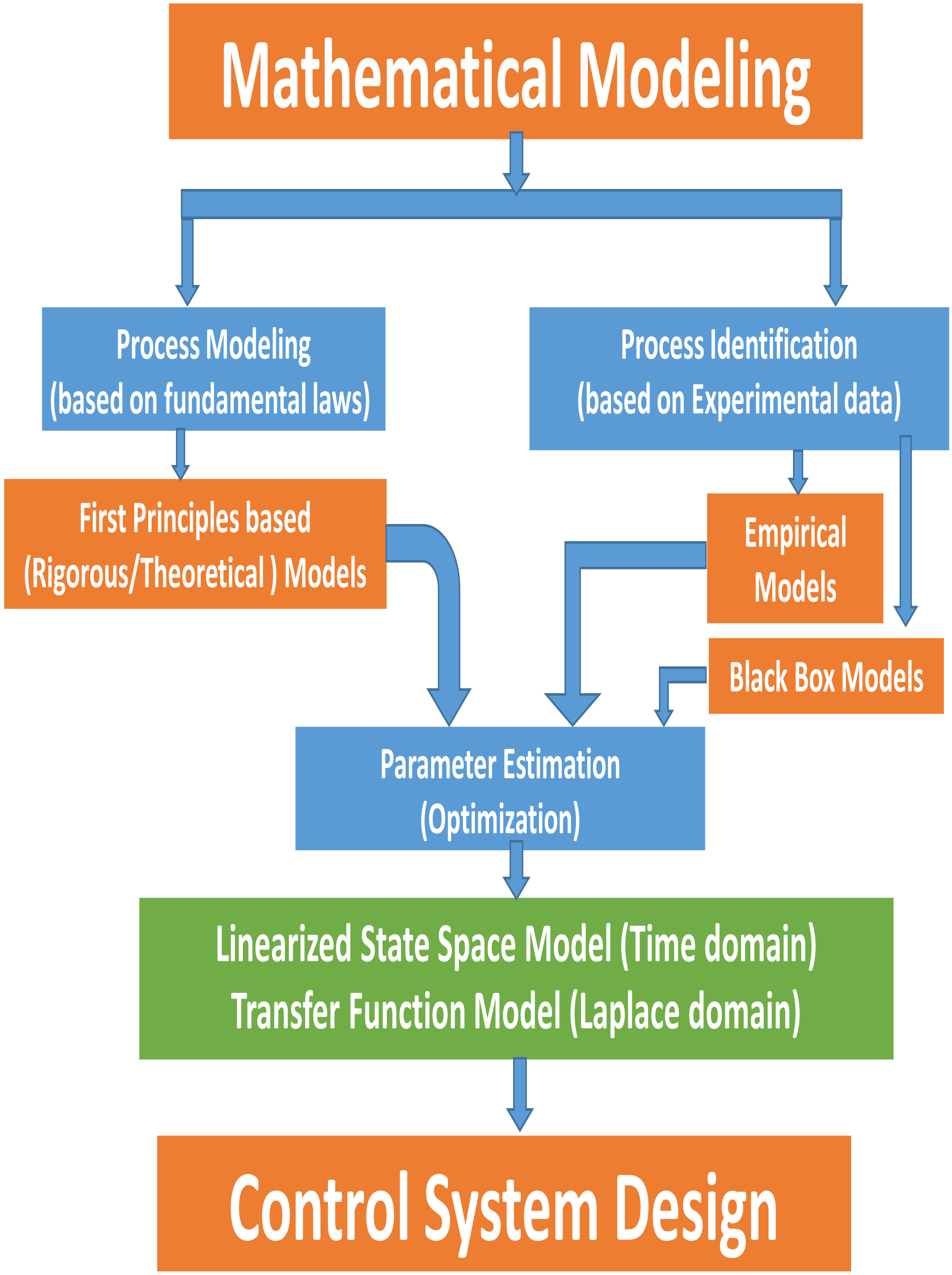

Figure 1. 1 Importance of Process Modeling and Identification in Control

1.4 Classification of Variables from the Process Control Perspective

For the design of control systems, it is utmost essential to have a clear classification of the different input variables, output variables and process parameters, as depicted in Figure 1.2. The classification of process variables and parameters is given as:

a) Input variables: These are further classified as manipulated variables and disturbance/load variables:

i. Manipulated variables (MV): These are the measured process variables whose values could be deliberately changed so that the controlled variables are maintained at their set-point values. Design of an efficient control system must ensure set point tracking property.

ii. Disturbance/load variables (DV): These are the input variables whose values are dictated by the external environment. These are measured (forcing functions) or unmeasured (process uncertainties). The disturbance variables may cause (undesirable) effect on the process such that the process may deviate from its desired (optimum) operating point. Design of an efficient control system must ensure that the effect of disturbances on the process is nullified (Disturbance rejection property).

b) Output variables: These are the measured process variables that are required to be controlled (hence are also known as controlled variables). The controlled variables (CV) are a subset of the process state variables.

c) Process parameters: In addition to the input and output variables, the process parameters have an important role to play in the control system design (Wang, 2020). It is essential in any control system design to have a good knowledge of the process parameters and the nature of their variation with time.

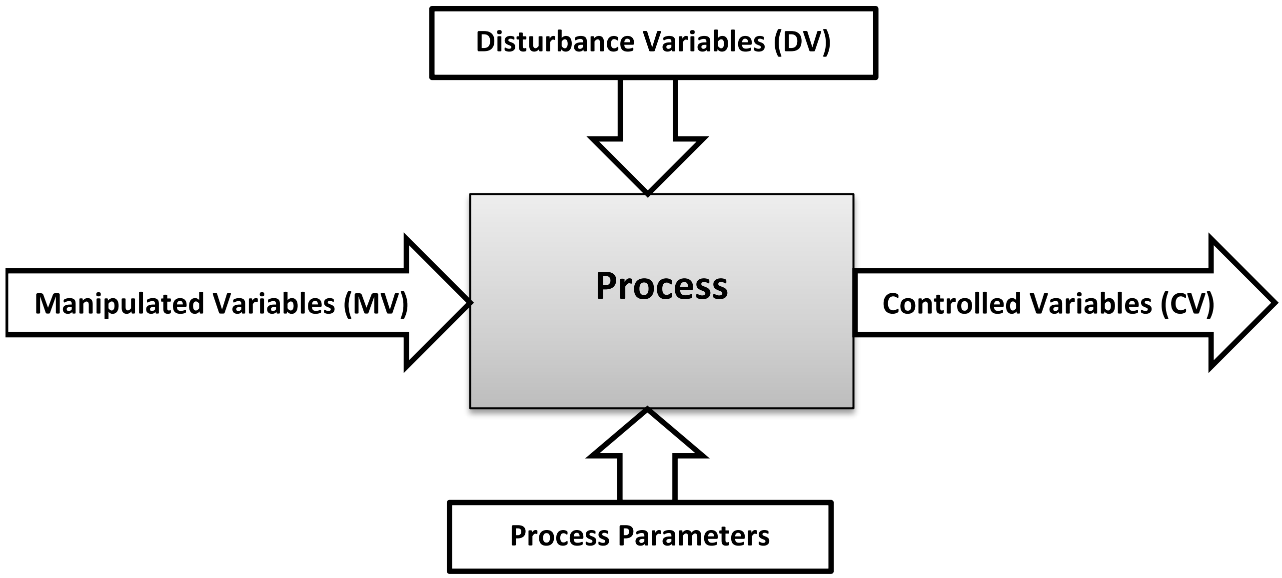

Figure 1. 2 Classification of variables from the Control perspective

1.5 Multivariable Process Control

Chemical processes that involve one controlled variable (CV) and one manipulated variable (MV) are termed as Single Input Single Output (SISO) systems. Such systems are relatively easier to control. But in practice, majority of important chemical processes require more than one output variable (CV) to be controlled simultaneously, using more than one input variable (MV), as shown in Figure 1.3. Such control problems are termed as Multiple Input Multiple Output (MIMO) control problems. The control of Multiple Input Multiple Output (MIMO) systems is challenging as these systems involve multiple control loops and process interactions among the control loops (Skogestad & Postlethwaite, 2005). A proper pairing among the controlled and manipulated variables (CV-MV pairing) becomes important.

1.5.1 Degrees of Freedom Analysis

Degrees of freedom analysis helps in identifying the number of control loops required for a process. A process is completely specified by reducing the number of degrees of freedom to zero. Mathematically, it is expressed as:

$$f = n_v - n_e \qquad \text{Eq. 1. 1}$$

where, f is the degrees of freedom of the process, n_v is the total number of variables in the process, and n_e is the total number of equations in the mathematical model of the process. Depending on the number of variables and equations, three situations are possible:

Case A: $f = 0$

When the number of variables is equal to the number of equations, the system is said to be completely specified. A unique solution can only be obtained by setting the degrees of freedom to zero.

Case B: $f < 0$

When the number of variables is less than the number of equations, the system is said to be over-determined. Such a case is usually encountered in optimization studies (Edgar et al., 2001); (Beveridge et al., 1970); (Ravindran et al., 2006); (Chong & Zak, 2010); (Fletcher, 2000).

Case C: $f > 0$

When the number of variables is more than the number of equations, the system is said to be under-determined. Such cases are more common in control system design.

There are two ways of reducing the degrees of freedom to zero: (i) by specifying the values of some of the input variables (forcing functions), and (ii) by writing additional (controller) equations: Controller equations represent mathematical (linear/nonlinear) functionality between a pair of controlled variable (CV) and manipulated variable (MV).

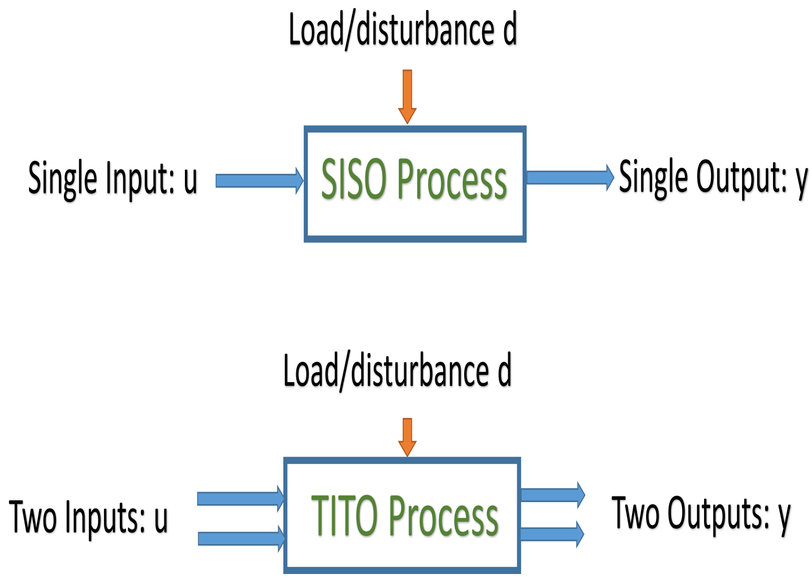

Figure 1. 3 Multivariable process control

1.6 Proportional Integral Derivative (PID) Feedback Control

The major advantage of the feedback control is that it does not require identification and measurement of the disturbances acting on the process. Moreover, since corrective action is based on the measured value of the process output, feedback control systems take care of the changes in process parameters and modeling errors. However, the feedback control system suffers from the major disadvantage that it does not take any corrective action until the process has felt the effects of any external disturbances and may eventually lead to closed loop instability.

Despite advances in the study of nonlinear control (Khalil, 2015), (Khalil, 2013), (Chidambaram, 1995), linear controllers have not lost their importance. Proportional Integral Derivative (PID) controller is most widely used in chemical process industries due to its fairly simple structure, robustness, vast range of applications, wide availability and standard hardware installation (Bequette, 1991). Nearly 97% of the regulatory controllers in the process industries employ PI/PID control algorithm (Shamsuzzoha, 2013; Wang et al., 2016). Closed loop block diagram of feedback control system is shown in Figure 1.4.

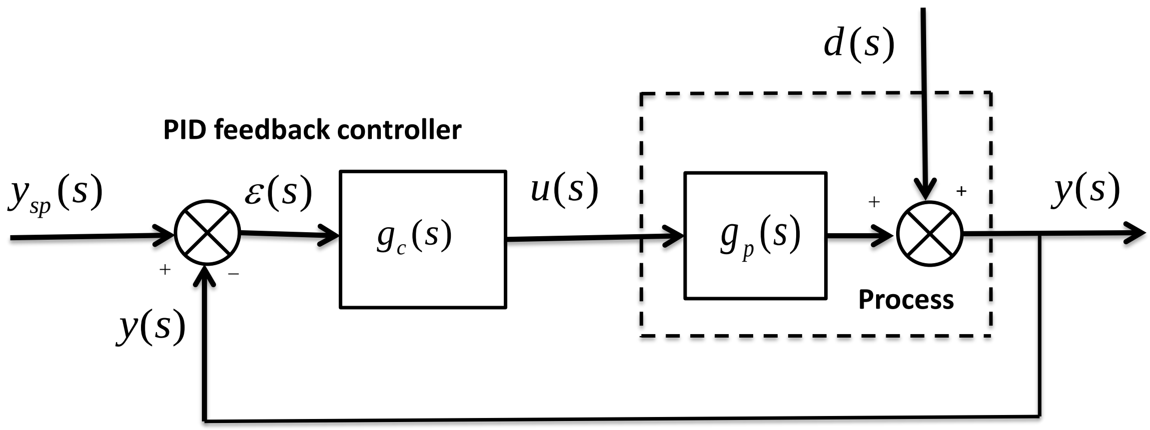

Figure 1. 4 Closed Loop Block Diagram of a PID Feedback Control System

1.7 PID Controller Design Methods

The PID controller design methods are broadly classified as conventional methods and Model based methods, as described in Table 1.1. The model based controller design methods provide better closed loop performance than the conventional design methods, in terms of quantitative performances indices (QPI) (Mokhatab & Poe, 2012), as described in Table 1.2.

Table 1. 1 PID Controller Design Methods

Controller Type	Design Method
Conventional PID controller	a) Ziegler-Nichols closed loop method b) Tyreus and Luyben closed loop method c) Ziegler-Nichols open loop method d) Cohen and Coon open loop method
Model based controller	a) Direct Synthesis (DS) method b) Internal Model Control (IMC) based PID control

Table 1. 2 Controller Performance Criteria (Quantitative Performance Index)

Process variable	Quantitative Performance Index (QPI)
Controlled variable (CV)	Integral of Square of Error (ISE) Integral of Absolute Error (IAE) Integral of Time Absolute Error (ITAE) Percentage overshoot (OS) One quarter decay ratio
Manipulated variable (MV)	Total Variation (TV)

The direct synthesis method and Internal Model Control (IMC) based PID method are the two classical model based controller design methods (Anil & Padma Sree, 2015; Begum et al., 2016; Krishna et al., 2012). In the direct synthesis method (Anil & Padma Sree, 2015), a desired closed loop response is selected and based on the knowledge of the process the best controller parameters are computed that may yield the desired response.

The Internal Model Control (IMC) method provides a strategy for the design of controller that uses the actual transfer function model of the process. This method has the following advantages (Bequette, 2003), (Smith & Corripio, 1997):

a) It can be implemented within the standard PID controller hardware framework (Johnson, 2015).

b) It involves only one tuning parameter instead of the three PID parameters (K_C, τ_I, τ_D) (Seborg et al., 2011).

1.8 Computer Simulation

Analytical solution to the set of mathematical equations may not be always available owing to the process nonlinearity. Simulation, in the engineering sense, is referred to as the numerical solution to a set of mathematical equations (process model), for a given set of inputs, using the appropriate numerical techniques (Constantinides & Mostoufi, 1999) , (Gupta, 2012) , (Yang et al., 2005) and a suitable computer programming language. Computer simulation provides the static (steady state) and dynamic (transient) response (behaviour) of the process, for a wide range of operating conditions.

1.8.1 Software Platforms

Some of widely used commercial and open source software applications that greatly help in the simulation studies are:

1. MATLAB and SIMULINK (Herniter, 2001), (Tewari, 2002)
2. Scilab

3. Microsoft Excel

4. Origin

1.8.2 Basic Types of Engineering Problems

The three basic types of engineering problems (as depicted in Figure 1.5) for which simulation studies are commonly carried out are:

1. Process Modeling/Identification/Optimization problem:

In the Process Modeling/Identification/Optimization problem, the unknown process model/system parameters are required to be estimated from the known/standard values of inputs and outputs.

2. Process control problem:

A process control problem aims at finding out the best values of the (unknown) input variables (Manipulated variables) for a well identified/known process with desired outputs (set points)

3. Process Dynamics (Servo/Regulator problem)

The simulation of a process dynamics problem aims at finding out the outputs of a well identified/known process, subjected to a given set of (known) inputs. The Process dynamics problem is further sub-classified as the Servo problem (study of closed loop responses to changes in set point) and Regulator problem (study of closed loop responses to load changes).

Type of Problem	Inputs u	Process G	Outputs Y
➢ Process Modeling & Identification	Known	Unknown ?	Known
➢ Process Control	Unknown ?	Known	Known
➢ Process Dynamics / Simulation • Servo Problem • Regulator Problem	Known	Known	Unknown ?

Figure 1. 5 Basic Types of Engineering Problems

1.9 General Objectives of the Present Work

As discussed above, most chemical and biochemical processes are multivariable processes. These are inherently nonlinear involving time-varying parameters and are prone to process uncertainties. Further, chemical and biochemical reactors are known to exhibit multiple steady states. The stability of the operating steady state plays an important role in the design of controller and simulation methodology. Model based PID controller design methods provide superior closed loop response as compared to the conventional methods. In view of these, following general objectives were set for this work:

a) Control of Multiple Input Multiple Output (MIMO) Processes

b) Control of Single Input Single Output (SISO) Stable Processes

c) Control of Single Input Single Output (SISO) Unstable Processes