1996


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ON-LINE STEADY-STATE GAIN IDENTIFICATION
FOR ON-LINE OPTIMIZATION OF MULTIVARIABLE
CONSTRAINED CHEMICAL PROCESSES

A Dissertation

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Louisiana State University and
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in

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by
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Abstract

The Amoco Model IV Fluidized Catalytic Cracking Unit (FCCU) (McFarlane et al, 1993) was augmented with Lee & Groves Model (1985) to provide for a simple but realistic product distribution model. This enabled a better and realistic on-line optimization of the FCCU. A Supervisory Multivariable Constrained Optimization (SMCO) algorithm was applied to this augmented model. It was observed that the FCC unit is optimized successfully, without violating any constraints. The parabolic error-penalizing function, incorporated in the algorithm allowed the constraints to asymptotically approach the limits without violating them. The on-line optimization to FCC unit led to maximizing of the feeds, reduction of reactor pressure and maximizing of the reactor temperature. The algorithm handled the benchmark disturbances very well by cutting down or increasing the manipulated variables as needed.

An On-line Steady-State Gain Identification (OSGI) method was developed to identify the steady-state gain matrix (SSGM) of any multivariable system. The SSGM is frequently used in multivariable control and/or on-line optimization. This method identifies the steady-state gains with all the controllers in the closed loop and thus can be implemented on-line. The use of the method was demonstrated in identification of SSGM for SMCO application for a CSTR. Two types of reactions were considered: irreversible and reversible reaction. The OSGI identified the drifting SSGM accurately for irreversible reaction. For the reversible reaction, OSGI was also employed to identify the cost-partials along with SSGM, which enabled the SMCO to track the drifting optimum with changing feed rate.
Chapter 1

Introduction

1.1 On-line Optimization

On-line optimization of a process compared to off-line, has a distinct advantage, in the inherent capability, to exploit the wealth of information springing continually from the process. This makes it able to cope with the process variability and redefine in context the optimal operating conditions. Chemical processes that are candidates for on-line optimization often involve complex reaction and separation systems and as such are typically multi-variable, interacting and non-linear. On-line optimization is frequently considered for plants where external disturbances are both relatively slow and have a significant impact on the optimum economic performance of the plant (Krishnan et al, 1992). Fluid Catalytic Cracking (FCC) is one of those processes. It is one of the most complex process units in an oil refinery with large reaction, fractionation and separation equipments. Their economic impact on refinery operation is also large. With large complex equipment, high throughputs and significant economic effects, these units present opportunities for advanced control and on-line closed loop optimization. A small improvement in the process through these techniques can result in significant gain. Depending on the particular unit, such a system can result in a $0.05 to $0.20/bbl improvement from advanced control, and $0.20 to $0.80/bbl from on-line optimization. For a modest FCCU of 25,000 bpd throughput this corresponds to an average $ 6 million per year (Lin, 1993).

McFarlane et al (1993) released a comprehensive and realistic industrial simulation system of a Model IV Fluidized Catalytic Cracking (FCC) process for academia and
industry alike to evaluate advanced control and on-line optimization schemes. The model is sufficiently complex to capture the major dynamic effects that occur in an actual system. However the model does not have any yield model for various fractions arising from cracking. It only gives a production of wet gas which is a function of reactor temperature alone. Lee & Groves (1985) model for FCC was coupled with this Amoco model to provide a simple yet effective yield model. The details of the combination will be given in Chapter 3. Supervisory Multivariable Control and Optimization (SMCO) by Daniel et al (1994) is applied to the process. The SMCO is also tested in presence of disturbances.

1.2 On-line Identification

A knowledge of open-loop process gain matrix for multivariable systems is necessary for the application of many well established control and analysis techniques. The availability of accurate steady-state gains for a multivariable process facilitates significantly the control system design procedure. Much information about the control properties of a multivariable process can be extracted from the steady-state gains of a process (Grosdidier et al, 1985).

Steady-state on-line optimization (Bamberger & Isserman, 1978; Mcfarlane & Bacon, 1989; Daniel et al, 1994) frequently employ a steady-state plant model using a steady-state gain matrix of the process. This steady-state gain matrix is usually identified around a nominal operating point. Process models are never perfect and because of unmodeled non-linearities or drifts with time, need modification from time to time. Frequently the operating conditions change and time varying parameters like catalyst deactivation, fouling factor of heat-exchangers, change in feed throughput, change. This in turn changes the gains associated with the process input and output variables. The steady-state gain matrix thus has to be updated on a regular basis. This can either be done in the traditional way of open-loop identification or using some later techniques of closed-loop
identification (Pensar & Waller, 1993; McIntosh & Mahalec, 1991; Melo & Friedly, 1992; Papastathopoulou & Luyben, 1990). However all these techniques are partially off-line techniques, and although the data is collected with the control loops closed, they do not update or identify the steady-state gain matrix on-line.

In response to this problem an on-line steady-state gain identification, OSGI for short, is developed and then applied to various processes to judge its performance. The on-line identification method should be simple enough for rapid computation on-line, yet sophisticated enough to handle multivariable processes. Since the identification of a steady-state gain matrix is the main motivation, only current steady-state samples of process inputs and outputs are needed.

The OSGI algorithm should be designed with move suppression, in order to restrict large changes in the steady-state gain matrix in a single sample. The method is essentially designed to track a drifting steady-state gain matrix caused by changes in operating conditions. Hence an initial start-up gain matrix is assumed to be known either through open-loop identification or through a priori knowledge of the transfer function matrix of the system. Since the OSGI method is designed essentially to enhance on-line optimization techniques, the stress will be given on application of OSGI for on-line optimization of constrained chemical processes. SMCO by Daniel et al (1994) will be used as the on-line optimization algorithm for the applications illustrated in this work.

1.3 Outline of the dissertation

In the next chapter, the literature is reviewed for on-line optimization of FCC units in the industry and academia. The on-line identification techniques used in control and on-line optimization are also reviewed. The similarities and the differences between the OSGI and other existing techniques are analysed. In Chapter 3, the process model simulator for
FCC is described. The Amoco model of the FCC (McFarlane et al, 1993) is supplemented with the Lee & Groves (1985) model for a better yield model. In Chapter 4, the application of SMCO to FCC process is described with implementation details in cost function, cost partials, constrained and manipulated variables etc. The SMCO optimization is studied and analyzed in the presence of disturbances to the system. In Chapter 5, the OSGI algorithm is proposed and details regarding the implementation, perturbation signal, etc. are discussed. The application of OSGI is illustrated for identification of steady-state gains for a simple binary distillation system. In Chapter 6, OSGI is applied to a CSTR to vividly describe the importance and efficacy of an on-line identification method in on-line optimization. Two types of reactions are illustrated: a reversible reaction and an irreversible reaction. Finally, the conclusions of the research and recommendations for future work are given in Chapter 7.
Chapter 2

Literature Review

2.1 On-line Optimization of FCCU

On-line optimization of the FCCU has traditionally been a challenge for a process/operations engineer due to its complexity and scope. Optimization of FCCU has been an active area of research in industry and academia alike (Kurihara, 1967; Schuldt & Smith, 1971; Prett & Gillette, 1980). Operators must decide to maximize fresh feed rate or reactor temperature, but not both. The strategy includes minimizing regenerator pressure, reactor pressure, and differential pressure, and maximizing feed rate, air blower capacity and reactor temperature (Lin, 1993).

McFarlane and Bacon (1989) demonstrated an adaptive optimizing control scheme for the FCC process. They did not model the reactor pressure or the differential pressure in their simulations. An empirical input-output model was used for recursive on-line identification and the steady-state information from the model was used for the steady-state optimization of the reactor-regenerator unit.

Rhemann et al (1989) reported on-line optimization of FCCU in Austria using a generalized reduced gradient (GRG) algorithm. IDENTification and COMmand (IDCOM) multi-variable predictive control was used for implementing the calculated optimal set-points. Fresh feed rate, heavy cycle oil (HCO) recycle rate, slurry recycle rate, reactor temperature and pre-heat temperature were used as the manipulated variables for optimization.
Lin (1993) used an equation based non-linear optimization system called simultaneous modular simulation. He enumerated benefits obtained from on-line optimization as: standard deviations of regenerator metallurgical temperatures decreased from 5-7 °C to 1.5-3 °C. This in turn increased reactor temperatures by 2-3 °C, resulting in higher conversion and better product quality. FCCU throughput increased by 3-9%. Standard deviation of naphtha endpoint decreased and higher naphtha production rates were achieved at the expense of light cycle oil (LCO).

Khandalekar and Riggs (1995) demonstrated a non-linear process model based control for the Amoco model IV FCC unit. The profit function was defined as the sum of the flow rates of all the product streams multiplied by their respective unit values, with the corresponding value of the feed subtracted from the sum. The cost of utilities (e.g. furnace fuel, regenerator air, etc.) was neglected. Also it was assumed that all the products formed had market demand. They also augmented the process model with Lee & Groves (1985) model to provide a yield model for gasoline, lighter-gas and gas-oil. Their steady-state optimization involves formation of steady-state models for gasoline yield, firebox, energy balances over reactor and regenerator and carbon yield. These steady-state balances were solved using Nelder-Mead optimization method (Riggs, 1988). The independent variables chosen were: reactor and regenerator temperatures, flue gas oxygen concentration and feed rate to the system.

The present work also has the same assumptions and profit function formulation. This work also combines Lee & Groves model with the Amoco model IV process for a better model of product yields. The difference is that a steady-state gain matrix is required as the model for SMCO which can be easily formed by step testing of manipulated variables. The manipulated variables chosen in this work are reactor temperature, reactor pressure and feed rate to the system. As shown later, lowering of the reactor pressure has more benefits.
in terms of blower capacities. Lower pressure also helps in the increased production of desirable higher octane products (McFarlane et al., 1993).

Recently Ellis and Riggs (1996) reported on-line optimization of the Amoco model IV (McFarlane et al., 1993) augmented by a ten lump yield model (Jacob et al., 1976 and Arbel et al., 1995). The steady-state optimization model and the independent variables were the same as Khandalekar and Riggs (1995).

2.2 On-line Identification

The goal in process identification is to infer a model (and estimates of the model parameters) given a data record. This activity can be carried out in an off-line manner, in which all data are analyzed at once, or by using on-line techniques, where the addition of new data point (or data set) is employed to update model parameters. Algorithms that are suited to real-time usage and are based on successive updating of the model parameters are called recursive, which use the previous sample estimates for prediction.

2.2.1 Recursive Least Squares (RLS)

There are a large number of recursive identification algorithms described in the literature (Ljung and Söderström, 1983); the most popular technique is recursive least squares (RLS), (Seborg et al., 1986).

A typical single-input single-output (SISO) model is usually described in the form of a linear difference equation, the so called ARMAX model, (Goodwin and Sin, 1984).
\[ y(t) + a_1 y(t-1) + \cdots + a_n y(t-n) = b_0 u(t-k) + b_1 u(t-k-1) + \cdots + b_m u(t-k-m) + c_0 \xi(t-1) + c_1 \xi(t-n) + \cdots + c_n \xi(t-n) + \epsilon(t) \]  

(2.1)

If the noise model parameters, \( c_i \), are set to zero, Eq. (2.1) can be written in the vector form as:

\[ y(t) = \psi^T(t-1) \theta(t-1) + \epsilon(t) \]  

(2.2)

where, information or regressor vector \( \psi \) is defined as:

\[ \psi^T(t-1) = [y(t-1), y(t-2), \ldots, y(t-n), u(t-k-1), \ldots, u(t-k-m-1), 1] \]

and parameter vector \( \theta \) is defined as:

\[ \theta^T = [a_1, a_2, \ldots, a_n, b_1, b_2, \ldots, b_m, d] \]

\( \epsilon(t) \) represents an error that is assumed to be statistically independent of the inputs and the outputs.

The equations for RLS computation of the unknown parameters are as follows (Clarke, 1981; Ljung and Söderström, 1983):

\[ \hat{\theta}(t) = \hat{\theta}(t-1) + K(t) [y(t) - \hat{y}(t)] \]  

(2.3)

where,

\[ \hat{y}(t) = \psi^T \hat{\theta}(t-1) \]  

(2.4)
\[ K(t) = \frac{P(t-1)\psi(t)}{1 + \psi^T(t)P(t-1)\psi(t)} \quad (2.5) \]

\[ P(t) = \left[ I - K(t)\psi^T(t) \right] P(t-1) \quad (2.6) \]

\( P \) is called the covariance matrix of the estimation error and \( K \) is the Kalman (feedback) filter gain.

Seborg et al, (1986), in their survey paper, discuss in detail the variations and modifications of the RLS and the practical solutions like covariance resetting, variable forgetting factor, perturbation signal to improve the performance of the RLS.

### 2.2.2 Instrumental Variable Method

When the noise is correlated with the process variable, instrumental variable (IV) is used instead of simple least squares. Using simple least squares leads to biased estimates. An instrument vector is formed consisting of instrument variables which are well correlated with \( \psi(t) \) but not correlated with the disturbance of the process. Both open-loop as well as closed loop IV methods exist in the literature. Ljung (1987) showed a four-step IV algorithm for open-loop systems described by an ARX (Auto Regressive Exogenous) model. Santos-Cordero (1995) proposed two closed-loop IV algorithms which are also implemented in a four step fashion. The algorithms showed comparable performances in the presence of white noise and correlated disturbances.

### 2.2.3 Projection Type Estimation Algorithms

Another class of estimation algorithm is projection type estimation algorithms. Goodwin et al, 1980 proposed a gradient algorithm:
\[ \dot{\theta}(t) = \dot{\theta}(t - 1) + \frac{\psi(t - 1)}{c + \psi(t - 1)^T \psi(t - 1)} \left[ y(t) - \psi(t - 1) \dot{\theta}(t - 1) \right] \quad (2.7) \]

For a multiple input multiple output (MIMO) case the algorithm becomes:

\[ \dot{\theta}_i(t) = \dot{\theta}_i(t - 1) + \frac{\psi_i(t - 1)}{c + \psi_i(t - 1)^T \psi_i(t - 1)} \left[ y_i(t) - \psi_i(t - 1) \dot{\theta}_i(t - 1) \right] \quad (2.8) \]

where,

\[ \psi_i^T(t - 1) = [y_i(t - 1), y_i(t - 2), \ldots, y_i(t - n), u_i^T(t - k - 1), \ldots, u_i^T(t - k - m - 1)] \]

and \( \dot{\theta}_i(t) \) is a \( (n_i + m(m_i + d_i)) \) vector of reals.

Seborg et al, (1986) proposed a slight variation in the above gradient algorithm:

\[ \dot{\theta}(t) = \dot{\theta}(t - 1) + \frac{\alpha(t) \psi(t - 1)}{1 + \alpha(t) \psi(t - 1)^T \psi(t - 1)} \left[ y(t) - \psi(t - 1) \dot{\theta}(t - 1) \right] \quad (2.9) \]

where \( \alpha(t) \) is a finite, non-negative, user-selected parameter that determines the speed of convergence. This parameter estimation law can be interpreted as follows: The new estimate \( \dot{\theta}(t - 1) \) is an orthogonal projection of \( \dot{\theta}(t - 1) \) onto the hyper-surface \( y(t) - \theta^T \psi(t - 1) = 0 \). The complete proof of convergence is given by Goodwin and Sin (1984).

The On-line Steady-state Gain Identification (OSGI) algorithm finds its inspiration from the algorithm described in section 2.2.3. It differs from the gradient algorithm with the fact that, OSGI uses only current steady-state data. Also in a multi-variable design (MIMO), OSGI forms a compact matrix instead of row wise updating as in the MIMO projection algorithm case.
Identification methods can be divided into non-parametric and parametric types. Parametric identification methods are primarily based on prescribed model forms and include parameter estimation methods for example. Non-parametric identification methods primarily yield forms such as frequency responses (Melo and Friedly, 1992). However, for closed-loop identification, non-parametric identification methods are not recommended, but instead parametric approaches, based on the prediction error method, enable either direct or indirect identification of the open-loop process (Söderström and Stoica, 1989).

2.3 On-line Identification in On-line Optimization

To deal with the non-linearities associated with the plant model over a wide range of operation, different approaches have been found in the literature. Prett & Gillette (1980) used a single step method of approximation programming (MAP) optimization. Instead of searching for a global optimum this method determines at regular time intervals the optimum operating point in a neighborhood of the current state. When this change is implemented and the process attains a new steady state, another such step towards the optimum is calculated. Each optimization change is calculated by linear program (LP) which uses a linearized (about current steady state operating point) process model.

Bamberger and Issermann (1978) demonstrated a method for adaptive on-line steady-state optimization of slow dynamic processes. Optimization information is obtained from the steady-state gain of an empirical dynamic process model identified on-line.

McFarlane and Bacon (1989) proposed an adaptive optimizing control scheme based on an empirical dynamic process model which is identified on-line using RLS. Dynamic information from the identified models was used for on-line updating of a multi-variable Internal Model Controller. Constrained steady-state optimization is accomplished using
the steady state information from the identified model in an on-line application of sectional linear programming. They demonstrated the method on a CSTR system and FCC unit.

Peterson and Whyatt (1989) developed an algorithm which uses RLS to identify a dynamic, discrete time model of a poorly defined system and used both the static and dynamic portions of the model for on-line optimization. They demonstrated the algorithm on a bioreactor simulation and reported that the dynamic information based optimization was found to be superior than the optimization based on the steady-state information of the identified model. However, dynamic optimization was suitable in bioreactor systems as it takes a very long time for the system to achieve a steady state. Steady state optimization is used in majority of the cases primarily because it allows the use of simple steady state models which are easy to develop and identify. The optimization problem is then solved at regular intervals (which is equivalent to the settling time of the process). The supervisory nature of the steady-state optimization also allows the usage of the existing control system as in most cases it only provides the optimal setpoints to the lower level controllers.

On-line parameter estimation is also used widely in identification of process models. The adjustable parameters in the model are identified and updated adaptively using a suitable method (Jang et al, 1986; Kiparissides et al, 1994; Khandalekar and Riggs, 1995).

Recently, there has been a widespread interest in usage of artificial intelligence (neural-network, genetic algorithms, etc.) based identification (Cheng et al, 1995; Cheng et al, 1996; Kristinsson and Dumont, 1992; Cox et al, 1996).

Daniel et al (1994) developed an on-line optimization algorithm (SMCO) using steady-state gain matrix as a plant model. This matrix is identified at a nominal operating point. However, for the model to be valid throughout the operating region of operation this steady-state gain matrix must be identified on-line in a closed loop fashion. Also SMCO requires that the cost-function must be expressed in terms of manipulated and constrained
variables. An on-line steady-state gain identification (OSGI) method is thus developed to achieve identification of the steady-state gain matrix (the process model) and to identify the cost partials with respect to the manipulated variables. This eliminates the requirement that the cost function be expressed in terms of the material and energy balances of the system. Thus a cost function can be formulated in any way. The initial values of the cost partials are given. OSGI performs a dual task:

1. It identifies the SSGM on-line as the process moves from one steady-state to another thus making the process model (SSGM) valid over the entire range of operation.

2. It also identifies the cost partials with respect to the manipulated variables which eliminates the tedious task of formulating the cost-function to incorporate the material and energy balances of the system.

2.4 Summary

In this chapter the FCCU on-line optimization results in industry and academia were presented. The on-line optimization of FCCU in this work was described and the similarities and the differences were highlighted. Literature review on the on-line identification techniques available was presented with the popular methods like, recursive least squares, projection algorithms and instrumental variable regression. A brief mathematical formulation of each method was given. On-line identification techniques used in on-line optimization applications were reviewed. Finally the similarities and the differences between the present work and the one in the literature were given.
Chapter 3

Fluidized Catalytic Cracking Unit

3.1 Introduction

The fluidized catalytic cracking (FCC) unit cracks heavier hydrocarbons into lighter and more valuable products. It receives multiple feeds consisting of high boiling point components from various parts of the refinery. Economic operation of the FCCUs plays an important role in the overall economic performance of the refinery. In most refineries, the operation of the FCCU is dictated by an off-line planning model, executed perhaps once a month. However, typically these planning models have relatively crude representations of actual FCCU operation. In addition, changes in unit constraints, operating conditions and economic incentives occur frequently (Rhemann et al, 1989). To capture these benefits, on-line optimization of the unit is required. An on-line optimization method called Supervisory Multivariable Constrained Optimization (SMCO) is to be applied to the FCC process model described by McFarlane et al, 1993. This model does not provide for any yield model or product distributions. Lee & Groves (1985) model is thus supplemented to the Amoco model (McFarlane et al, 1993) to provide for a yield model which gives product distribution. Next section describes the operation of Model IV FCC unit.

3.2 Model IV FCCU

Fig. 3.1 shows the process flow diagram of a model IV FCC unit. Pre-heated feed is mixed with hot slurry recycle from the bottom of the main fractionator and injected at the bottom of the riser along with the hot catalyst from the regenerator. This totally vaporizes
Figure 3.1: Schematic of Model IV FCC process

the feed. The hot catalyst provides the sensible heat, the heat of vaporization and the heat of reaction necessary for the endothermic cracking reaction. In the reactor, coke is deposited on the catalyst and hence catalyst has to be regenerated in the regenerator by burning off the coke in presence of air. The air is provided to the regenerator by two centrifugal air blowers the combustion air blower (which provides the bulk air) and the lift air blower (which also assists in altering the density of the catalyst for circulation). Reactor product gas is passed to the main fractionator for heat recovery and separation into various products.
Spent catalyst is transported back to the regenerator through a U-bend tube. Air is injected at the bottom of the regenerator lift pipe to assist in the circulation of the catalyst. Catalyst in the regenerator is fluidized using the air from the lift and combustion air blowers. Carbon and hydrogen on the catalyst react with the air to form carbon monoxide, carbon-dioxide and water. The flue gas travels up the regenerator through the cyclones where entrained catalyst is removed. Regenerated catalyst flows over a weir into the regenerator stand pipe. The level of the catalyst in the stand-pipe provides the driving force for the catalyst flow back to the reactor.

3.3 Amoco Model

The dynamic simulator for the model IV FCC process was adopted from the extensive mathematical model provided by McFarlane et al (1993). The set of time dependent ordinary differential equations were integrated using fourth-order Runge-Kutta method. The Amoco model does not provide any yield model and the product of cracking is assumed to be only wet gas and coke. The wet gas is assumed to be a function of only reactor temperature. The reactor itself is modeled in a simplified manner. The yield of wet gas is given as:

\[ F_{wg} = (F_3 + F_4) \left[C_1 + C_2(T_r - T_{ref})\right] \] (3.1)

where, \(C_1\) and \(C_2\) are empirical constants and,

- \(F_{wg}\) wet gas production in reactor (mol/s)
- \(F_3\) Flow of fresh feed to reactor riser (lb/s)
- \(F_4\) Flow of slurry to reactor riser (lb/s)
- \(T_r\) Temperature of reactor riser (°F)
- \(T_{ref}\) Base temperature for energy balance (°F)
The riser energy balance assumes stirred tank dynamics, with negligible heat loss to the environment. The heat of cracking is simply assumed to be proportional to the riser temperature. The detail model is given in Appendix B.

The spatial differential equations for the regenerator are integrated once every three steps in the time domain without losing significant accuracy. This sped up the computation time considerably.

3.4 Lee & Groves Model (1985)

The model uses the three lump model of Weekman et al (1970) to describe the kinetics of the system. Shah et al (1977) extended Weekman’s results to account for cracking in a transfer line under adiabatic, endothermic condition. The chemical species are combined or lumped into three pseudo-components: gas-oil, gasoline, and light gases/carbon. The reactions are represented by:

Reaction 1: \[ F \xrightarrow{k_1} G + L \]
Reaction 2: \[ G \xrightarrow{k_2} L \]

where F is feed = gas oil, G = gasoline and L = light gases/carbon. Gasoline is the most valuable product in the cracking. The production of gasoline is the desired reaction; however, cracking of feed to lighter products and over-cracking of gasoline to lighter products are the undesired reactions. The model treats the riser as an adiabatic plug flow reactor. It is a quasi-steady state model in the sense that it neglects changes with time during passage of feed through the riser. Since the residence time of the feed in the riser is less than 10 seconds, and the characteristic time for changes in the regenerator is on the order of hours, this is a reasonable approximation. The model consists of the following material and energy balances:
Material balance on gas-oil

\[
\frac{dy_f}{dz} = -R^0_r [COR] \Phi_0 \Phi_0^2 \exp \left( -\frac{E_f}{RT_0(1 + \theta)} \right) \exp(\alpha r z) \quad (3.2)
\]

Material balance on gasoline

\[
\frac{dy_g}{dz} = R^1_r [COR] \Phi_0 \Phi_0^2 \exp \left( -\frac{E_f}{RT_0(1 + \theta)} \right) \exp(\alpha r z) - R^0_g [COR] \Phi_0 \Phi_0^2 \exp \left( -\frac{E_g}{RT_0(1 + \theta)} \right) \exp(\alpha r z) \quad (3.3)
\]

Energy balance (assuming adiabatic operation)

\[
\frac{d\theta}{dz} = \frac{\lambda \Delta H_f F_0}{T_0(F_s C_{Ps} + \lambda F_0 C_{Po} + (1 - \lambda) F_D C_{Po})} \frac{dy_f}{dz} \quad (3.4)
\]

The weight fraction of light gases is thus \(1 - y_g - y_f\). The initial activity \(\Phi_0\) of the catalyst at the inlet to the reactor was assumed to be linearly related to carbon on regenerated catalyst as \(\Phi_0 = 1 - mG_{RC}\). The nomenclature for the symbols used is given below:

\begin{align*}
COR & \quad \text{Catalyst to oil ratio} \\
C_{Ps} & \quad \text{Heat capacity of dispersing steam} \\
C_{Po} & \quad \text{Heat capacity of oil} \\
C_{Ps} & \quad \text{Heat capacity of catalyst} \\
G_{RC} & \quad \text{Weight percent of coke on regenerated catalyst} \\
E_f & \quad \text{Activation energy for gas oil cracking} \\
E_g & \quad \text{Activation energy for gasoline cracking} \\
F_D & \quad \text{Flow of steam} \\
F_O & \quad \text{Flow of oil}
\end{align*}
For more details on the model the reader should refer to Lee & Groves (1985).

3.5 Combination

The reactor riser model described above is added to the Amoco model to get an approximate yet realistic distribution of products. The simple yield model described by Eqn. (3.1) is replaced by the reactor riser model described in the preceding section. However, the...
Amoco model is used to predict the coke yield from cracking. The yield of coke is thus subtracted from the yield of lighter gases/carbon as predicted by the Lee and Groves model. For every time step in the integration of the Amoco model the equations (3.2), (3.3) & (3.4) are integrated using Runge-Kutta fourth order method to yield the product fractions. The model gives a temperature distribution along the length of the reactor riser. The Amoco model assumes stirred tank dynamics for riser energy balance. A difference was observed between the temperature predicted by the Amoco model and the temperature predicted by the Lee & Groves model. The average reactor riser temperature was therefore calculated as (Khandalekar & Riggs, 1995):

\[ T_{\text{riser}} = 0.3T_{\text{inlet}} + 0.7T_{\text{out}} \]  

(3.5)

This exactly matched the riser temperatures predicted by both the models.

### 3.6 Control and Optimization Scheme for FCCU

Fig. 3.2 shows the control structure adopted for the system. The regulatory control structure was adopted from Linares (1994). As shown, the reactor pressure is controlled by manipulating the wet gas compressor suction valve. The carbon-monoxide stack gas controller (AC-1) is cascaded with a flow controller (FC-1) which manipulates the lift air blower speed. The total air supplied to the regenerator is the input to the flow controller FC-1. Linares (1994) in his scheme had the flow controller (FC-1) manipulate the combustion air blower suction valve and the lift air blower speed was set at a constant value. However the disadvantage of that scheme was that the valve saturated too often, thus limiting the flow of total air to the regenerator. The flow controller (FC-1) was retuned with the changed manipulated variable. The reset time was adjusted until an adequate
The reactor temperature controller (TC-1) is cascaded with a differential pressure controller (dPC-1) which manipulates the stack gas valve, to change the differential pressure between the reactor and the regenerator. Any change in the differential pressure controller (dPC-1) setting affects the catalyst circulation rate and affects the temperature of the reactor. The regenerator temperature is controlled by manipulating the flow rate of recycle slurry from the main fractionator. However the controller for the regenerator

Figure 3.2: Control and SMCO optimization scheme for FCCU

response was achieved and then the controller gain was adjusted to obtain the desired performance.
temperature (TC-2) takes action only above a certain pre-determined threshold limit. Below the limit the regenerator temperature is in open loop. This is possible because the regenerator temperature response is very slow to any disturbances. A flow controller (FC-2) is also employed to manipulate the flow of fresh feed to the reactor riser.

3.7 Summary

In this chapter, an overview of Model IV FCC process is given. The main purpose of this chapter is to demonstrate the combination of the two dynamic mathematical models by McFarlane et al (1993) and Lee & Groves (1985). The Amoco model by McFarlane et al (1993) does not provide any yield model and the products of cracking are assumed to be only wet gas and coke. Lee & Groves model is combined with this model to provide a simple yet realistic yield model which provides for cracking of feed into gasoline and lighter gases using a three lump model.

The control structure for this model is described and the controlled and manipulated variables are identified. This control system acts as the low level regulatory control scheme for the supervisory control and on-line optimization scheme described in the next chapter. The next chapter demonstrates the application of SMCO (Daniel et al, 1994) to this process. The results obtained are analyzed. Benchmark disturbances are also applied to the FCC unit to test the SMCO.
Chapter 4

Application of SMCO to FCCU

4.1 Introduction

Supervisory Multivariable Constrained Optimization (SMCO) algorithm (Daniel et al., 1994) is applied to the FCC process model described in Chapter 3. This algorithm was chosen over the other algorithms because it allows efficient utilization of computer resources. The general formulation of the cost function is allowed in terms of real cost terms. It also has an advantage of smooth integration of constraint enforcement and cost minimization. Its simplicity, compactness and yet effective application make it an attractive choice. The overhead required in terms of designing and implementing the application to any process are also minimum. The algorithm minimizes an objective function that combines process constraints, move suppression terms and a cost function. Such a function with N constrained variables and M manipulated variables can be written as:

\[
J = \sum_{i=1}^{N} (w_i E_i)^2 + \sum_{j=1}^{M} \lambda_j (\Delta u_j)^2 + w_c C(y, u)
\]  \hspace{1cm} (4.1)

subject to:

\[
y_i = y_i^0 + \sum_{j=1}^{M} a_{ij} \Delta u_j
\]  \hspace{1cm} (4.2)

where all variables are defined in Appendix A. The first term is the weighted sum of squared errors \((E_i)\), which represents the constraints on the dependent variables \((y_i)\). The second term is the weighted sum of control moves (usually controller setpoints) squared. \(\lambda_j\) is the move suppression parameter which limits any large change in the moves. The
last expression in the objective function is the cost function. The imposed condition in Eqn. (4.2) is just a steady-state model where \( y^0 \) is the current measurement of the process output and \( a_{ij} \) is the appropriate steady-state gain between manipulated variable \( u_j \) and output \( y_i \). The above objective function is minimized using least-squares approach. This yields the basic equation which calculates the controller moves:

\[
\Delta u = \left[ A^T W^T W A \otimes (I + \Lambda) \right]^{-1} \left[ A^T W^T W E - \frac{1}{2} w_c \frac{DC}{D\Delta u} \right] \tag{4.3}
\]

It can be viewed in simpler terms as a control term and cost term.

\[
\Delta u = K_c E - K \frac{DC}{D\Delta u} \tag{4.4}
\]

where \( K_c \) represents controller gain and \( K \) represents cost gain.

The cost differential in Eqn. (4.3) can be expressed as:

\[
\frac{DC}{D\Delta u_k} = \frac{\partial C}{\partial \Delta u_k} + \sum_{i=1}^{N} \frac{\partial C}{\partial y_i} \frac{\partial y_i}{\partial \Delta u_k} = \frac{\partial C}{\partial \Delta u_k} + \sum_{i=1}^{N} \frac{\partial C}{\partial y_i} a_{ik} \quad k = 1 \ldots N \tag{4.5}
\]

where steady-state relation in Eqn. (4.2) has been used. The error on the constrained variables \((y_i)\) is defined as:

\[
E_i = y_{i}^{\text{set}} - y_i = y_{i}^{\text{set}} - y_i^0 - \sum_{j=1}^{M} a_{ij} \Delta u_j = E_i^0 - \sum_{j=1}^{M} a_{ij} \Delta u_j \tag{4.6}
\]

where \( y_{i}^{\text{set}} \) is the desired value of the constrained variable \( y_i \). SMCO includes the constraints via the error term \((E)\) in the Eqn. (4.3). The error term is defined as the midpoint of the constrained range minus the current output \((E = Y_{\text{mid}} - Y)\). The error is thus
symmetrically distributed around the midpoint of a valid range. The error term is modified by a parabolic penalty function \( f = cE^2 \) as shown in Figure 4.1. When the variable is outside its constraints the penalty factor \( f \) is set to unity. The penalty factors are used to modify the midpoint errors \( E'_i = f_i \times E_i \) used in the control move calculation. With this penalized error \( E'_i \), the error term is de-emphasized near its midpoint and emphasized near the constraint borders, allowing the algorithm enough freedom to find a minimum and to take action before the constraint is violated. Thus variables get increasingly penalized as they approach the constraints.

![Parabolic Penalty Functions for Error](image)

**Figure 4.1: Penalty Functions for Error**

The three major steps involved in implementation of SMCO to any process are (Daniel, 1994):

1. Terms such as constrained errors, cost, gains and cost partials must be calculated for the process to be optimized.

2. A routine which follows Eq. (4.3) must be written to use the values calculated above and calculate the optimum controller moves.
3. The optimum control moves must be processed and passed on to the lower level controllers.

### 4.2 Constrained and Manipulated Variables

A detailed list of constraints is given in McFarlane et al, 1993. The constraints of importance which are chosen in this application are:

<table>
<thead>
<tr>
<th>Constrained Variables</th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>Level of catalyst in stand-pipe, ft</td>
<td>10.0</td>
<td>( L_{sp} ) 20.0*</td>
</tr>
<tr>
<td>Diff. bet. cyclone and regen. bed temp., °F</td>
<td>10.0</td>
<td>( T_{\text{diff}} ) 20.0*</td>
</tr>
<tr>
<td>Regenerator temperature, °F</td>
<td>1260.0</td>
<td>( T_{\text{reg}} ) 1290.0*</td>
</tr>
<tr>
<td>Regenerator pressure, psi</td>
<td>20.0</td>
<td>( P_e ) 39.7*</td>
</tr>
<tr>
<td>Governor setpoint of the lift air blower</td>
<td>0.45</td>
<td>( V_{lift} ) 0.65*</td>
</tr>
<tr>
<td>Wet gas compr. suction valve position</td>
<td>0.85</td>
<td>( V_{11} ) 0.95*</td>
</tr>
</tbody>
</table>

*McFarlane et al (1993)*

The minimum constraint limit value is chosen such that the normal operating point of the variable is at the midpoint of the constrained range, e.g. the \( L_{sp} \) has a normal operating value of approximately 15 ft. The combustion air blower is operated at full capacity (suction valve \( V_6 \) fully open) and the lift air blower speed of 5700 rpm at normal operation. This corresponds to the governor setpoint of 0.65. The air blower speed can be increased to 6320 rpm to respond to disturbances. The suction valve on the wet gas compressor is 95% open \( (V_{11} = 0.95) \), its desired operating point (McFarlane et al, 1993).

Carbon-monoxide stack gas concentration (COSG) is also an important constraint in the system. McFarlane et al (1993) describe two types of combustion constraints:

- **set A**: \( C_{O_2,sg} > 1.5\% \quad T_{\text{reg}} \geq 1265°F \)
- **set B**: \( T_{\text{diff}} = T_{\text{cyc}} - T_{\text{reg}} \leq 20°F \quad C_{CO,sg} \leq 350 \text{ ppm} \)
The set B is implemented in this work. Initially COSG was included as one of the constrained variables, however it was noticed that the regulatory controllers (AC-1 and FC-1) held the COSG concentration at its setpoint, and the constraint was never violated. The manipulated variable (the lift air blower speed, $V_{u1}$) did go past its normal operating point of 0.65 (5300 rpm), while maintaining the setpoint. Thus the constrained variables which were controlled by regulatory controllers were taken off the constrained variable list of SMCO; instead they were implemented indirectly by letting the lower level regulatory controller control the variable, and the manipulated variable of the controller was included as the constrained variable. For example, COSG controller (AC-1) is the low level regulatory controller which controls COSG while $V_{u1}$ is included as the constrained variable for SMCO. The other constraints like $T_r \leq 995^\circ F$ and $P_4 < 49.2$ psig could be easily implemented as they are the constraints on the manipulated variables of SMCO.

As mentioned in Chapter 2, the FCC unit is usually optimized by one or more of the following combinations: increasing feed-throughput, increasing reactor temperature, decreasing reactor/regenerator pressure, maximizing air blower capacity and decreasing differential pressure. Thus the manipulated variables for the SMCO are selected as:

<table>
<thead>
<tr>
<th>Manipulated Variables</th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow of gas-oil feed to the reactor riser, lb/s</td>
<td>118.0</td>
<td>130.0</td>
</tr>
<tr>
<td>Reactor pressure setpoint, psi</td>
<td>30.0</td>
<td>36.0</td>
</tr>
<tr>
<td>Reactor temperature setpoint, °F</td>
<td>985.0</td>
<td>995.0*</td>
</tr>
</tbody>
</table>

* McFarlane et al (1993)

The SMCO algorithm uses the steady-state gain matrix between the constrained and manipulated variables as the process model. It is initially formed by making a step change in each of the manipulated variables and recording the change in the constrained variables.
while keeping the other manipulated variables constant. Table 4.3 shows the SSGM formed for this application.

Table 4.3: Steady State Gain Matrix (SSGM) for FCCU

<table>
<thead>
<tr>
<th></th>
<th>$F_3^{set}$</th>
<th>$T_4^{set}$</th>
<th>$T_r^{set}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_{sp}$, ft</td>
<td>0.52</td>
<td>0.84</td>
<td>0.120</td>
</tr>
<tr>
<td>$T_{diff}$, °F</td>
<td>0.02</td>
<td>0.40</td>
<td>-0.125</td>
</tr>
<tr>
<td>$P_5$, psig</td>
<td>-0.06</td>
<td>0.76</td>
<td>0.01</td>
</tr>
<tr>
<td>$T_{reg}$, °F</td>
<td>-1.46</td>
<td>0.36</td>
<td>0.56</td>
</tr>
<tr>
<td>$V_{in}$</td>
<td>0.08</td>
<td>0.48</td>
<td>0.04</td>
</tr>
<tr>
<td>$V_{11}$, fraction open</td>
<td>0.02</td>
<td>-0.12</td>
<td>0.00</td>
</tr>
</tbody>
</table>

These gains are the changes in the constrained variables per unit change in each of the manipulated variables. For example, the gain $\frac{\partial L_{sp}}{\partial F_3^{set}} = 0.52$ ft/lb/s is the resulting change in stand-pipe level, per unit increase in the flow rate of the feed $F_3$, while keeping the reactor pressure ($P_4$) and reactor temperature ($T_r$) constant. The reactor pressure controller and the reactor temperature controller were kept in AUTO mode and a unit step change was made in the feed flow rate setpoint ($F_3^{set}$) while the process was operating at a steady state. After reaching a new steady state, the change in each of the constrained variables was recorded. This forms the first column of the Table 4.3. Other columns were formed in a similar fashion.

4.3 Cost Function

The cost function or objective function is defined as the difference between the value of the feed and that of the products. In other words the feed streams are multiplied by their unit values and the value of product streams multiplied by their unit values is subtracted from it. The cost of utilities (e.g. fuel oil, regenerator air etc.) are neglected. The feed is made up of gas-oil, diesel, wash-oil and a little amount of recycled slurry. There is no
diesel or wash oil added to the feed in this work. The cost of slurry is neglected. Also, it is assumed that all the products have market demand. The unused feed (gas-oil) is assumed to be completely recovered and thus has a product value.

\[ C = F_3 v_3 - (F_{gl} v_{gl} + F_{gs} v_{gs} + F_{ugo} v_3) \]  

(4.7)

Cost partials with respect to manipulated variables are straightforward but require the partials of \( F_3, F_{gl}, F_{gs} \) and \( F_{ugo} \) with respect to the manipulated variables and are given as:

Table 4.4: Cost partials for SMCO application to FCCU

<table>
<thead>
<tr>
<th>( \partial )</th>
<th>( \partial F_3^{set} )</th>
<th>( \partial F_{gl}^{set} )</th>
<th>( \partial F_{gs}^{set} )</th>
<th>( \partial F_{ugo}^{set} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \partial F_3 )</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>( \partial F_{gl} )</td>
<td>0.4109</td>
<td>0.0</td>
<td>0.0019(( F_3 + F_4 ))</td>
<td>0.0015F_3 +F_4</td>
</tr>
<tr>
<td>( \partial F_{gs} )</td>
<td>0.1773</td>
<td>0.0</td>
<td>0.0015(( F_3 + F_4 ))</td>
<td>0.0034F_3 +F_4</td>
</tr>
<tr>
<td>( \partial F_{ugo} )</td>
<td>0.4118</td>
<td>0.0</td>
<td>-0.0034(( F_3 + F_4 ))</td>
<td></td>
</tr>
</tbody>
</table>

This table was obtained in a similar fashion as the SSGM calculation described in the earlier section. It is obtained by step testing each manipulated variable while holding the other manipulated variables constant. For example, \( \partial F_{gl}/\partial F_3^{set} = 0.4109 \) lb/s per lb/s is the resulting change in the gasoline flow, per unit increase in the flow of feed (gas-oil) while holding reactor pressure (\( P_4 \)) and reactor temperature (\( T_r \)) constant. \( \partial F_{gl}/\partial T_r^{set} = 0.0019(\( F_3 + F_4 \)) \) lb/s per °F is the resulting change in the gasoline flow per unit increase in the feed flow rate. The partial with respect to reactor temperature (\( T_r \)) is this way because Lee & Groves (1985) model gives yield in terms of weight fraction of gasoline.

A gain of zero (e.g. \( \partial F_{gl}/\partial P_4^{set} \)) means there is no change in the variable per unit increase/decrease in the manipulated variable or in other words the manipulated variable...
has no influence on that variable. Table 4.5 contains the unit values and densities of gas-oil, gasoline and lighter gas.

Table 4.5: Densities and unit values for feed and product streams for FCCU

<table>
<thead>
<tr>
<th>Density in API</th>
<th>Value per gal</th>
</tr>
</thead>
<tbody>
<tr>
<td>F₃</td>
<td>27</td>
</tr>
<tr>
<td>F₄</td>
<td>20</td>
</tr>
<tr>
<td>F₁₆</td>
<td>57</td>
</tr>
<tr>
<td>F₂₄</td>
<td>220</td>
</tr>
<tr>
<td>F₂₄₉</td>
<td>24</td>
</tr>
</tbody>
</table>

† Gary and Handwerk (1994) ‡ Khandalekar and Riggs (1995)

4.4 Implementation

The simulation was developed and programmed in C++ on Unix. A function was written based on Eq. (4.3) to calculate the optimal setpoints for the controllers described in Chapter 3. The FCC model equations and the reactor riser equations were integrated using Runge-Kutta fourth order method. The value of the move suppression parameter ($\lambda$) and the cost term weighting factor ($w_c$) in Eq. (4.3) were determined by trial and error by keeping the optimizer in open-loop; i.e. not passing the optimal setpoints to the controllers on-line but observing them in an off-line manner.

The $\lambda$ is a scalar parameter and was tuned to achieve a reasonable size change from one steady-state to another. The $\Lambda$ is a diagonal matrix with $\lambda$ as its diagonal elements. The $\lambda$ was tuned such that the optimal control moves are not very large and are approximately 0.5-1% of the total range of the respective manipulated variable. The addition of $(I + \Lambda)$ to the diagonal elements of the $A^TW^TWA$ in Eqn. (4.3) ensures the same amount of move suppression to all the manipulated variables. The $w_c$ was tuned till the plant could
be operated comfortably close to the constraints without violating any of them. The $\lambda$ was decided to be 0.5 and $w_c$ was fixed as 0.75.

4.5 Simulation Results

A base case with the initial conditions as given in Table 4.6 was chosen. The process was then subjected to on-line optimization by SMCO and was allowed to move to a new steady state until no further optimization was observed. The final values at this steady-state were stored. This state is referred to as optimal state. The process conditions at the optimal state are given in Table 4.8. The FCC process at this optimal state was further subjected to different types of disturbances to study the response of SMCO to these disturbances. The conditions at the optimal state were used as the initial conditions for studying disturbances to the system.

Table 4.6: FCCU On-line Optimization: Initial Conditions, Base State

<table>
<thead>
<tr>
<th>$L_{ap}$</th>
<th>12.3 ft</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{diff}$</td>
<td>14.13 °F</td>
</tr>
<tr>
<td>$T_{rel}$</td>
<td>1276.5°F</td>
</tr>
<tr>
<td>$P_6$</td>
<td>29.6 psig</td>
</tr>
<tr>
<td>$V_{lift}$</td>
<td>0.37</td>
</tr>
<tr>
<td>$V_{ll}$</td>
<td>0.85</td>
</tr>
<tr>
<td>$T_{feed}$</td>
<td>460.9 °F</td>
</tr>
<tr>
<td>$T_{amb}$</td>
<td>75 °F</td>
</tr>
<tr>
<td>$\psi$</td>
<td>1.00</td>
</tr>
<tr>
<td>AC-1$^{\text{set}}$</td>
<td>300 ppm</td>
</tr>
<tr>
<td>FC-1$^{\text{set}}$</td>
<td>78.21 lb/s</td>
</tr>
<tr>
<td>TC-1$^{\text{set}}$</td>
<td>991.0 °F</td>
</tr>
<tr>
<td>dPC-1$^{\text{set}}$</td>
<td>-3.58 psig</td>
</tr>
<tr>
<td>TC-2$^{\text{set}}$</td>
<td>1276.5 °F</td>
</tr>
<tr>
<td>FC-2$^{\text{set}}$</td>
<td>122.0 lb/s</td>
</tr>
<tr>
<td>PC-1$^{\text{set}}$</td>
<td>33.14 psia</td>
</tr>
</tbody>
</table>
Table 4.7: Summary of FCCU optimization

<table>
<thead>
<tr>
<th>Feed (API)</th>
<th>Case</th>
<th>( F_3 ) (lb/s)</th>
<th>( P_4 ) (psi)</th>
<th>( T_r ) (° F)</th>
<th>( \Delta ) Obj. Fcn.</th>
</tr>
</thead>
<tbody>
<tr>
<td>27</td>
<td>Base</td>
<td>122.00</td>
<td>33.14</td>
<td>991.0</td>
<td>-</td>
</tr>
<tr>
<td>27</td>
<td>Optimal</td>
<td>124.62</td>
<td>32.94</td>
<td>995.0</td>
<td>$6000/day</td>
</tr>
</tbody>
</table>

4.5.1 On-line Optimization

Figure 4.2 and 4.3 show the response of the constrained variables and the manipulated variables to the on-line optimization. The SMCO is switched on after 10 minutes of normal running of the operation. As seen in Figure 4.3(a) the SMCO increases the flow of gas-oil feed to increase production rate. The riser temperature is also increased, (Figure 4.3c) as a significant economic incentive lies in doing so, as shown by the cost partials in Table 4.4. The partials for gasoline \( (F_{gi}) \) and light gas \( (F_{gt}) \), with respect to reactor temperature, are positive, meaning any increase in reactor temperature \( (T_r) \) will result in increased production of gasoline and light gas, which is desirable. An increase in feed flow rate and reactor temperature, increases the production rate and also the deposition of carbon on the catalyst. This additional carbon has to be burnt off in the regenerator. The air flow rate to the regenerator thus has to be increased. Controller AC-1 demands for additional air supply which is complied by the flow controller FC-1, by increasing the speed of the lift air blower (Figure 4.2e).

Higher reactor pressures reflect in higher regenerator pressures because \( dPC-1 \) controller maintains a constant differential pressure between reactor and regenerator. These higher regenerator pressures increase the polytropic heads of the air blowers, reducing air blower throughput (McFarlane et al, 1993). Thus it is advantageous to reduce the reactor pressure to reduce the polytropic head of the lift air blower. As seen from Table 4.3 this increase in the lift air blower speed towards its upper constraint can be offset by...
decreasing the reactor pressure setpoint. In SMCO, the error caused by increase in lift air blower speed \((V_{lift})\) towards its constraint is penalized by the parabolic penalty function as described in the beginning of this chapter. The control term in Eqn. (4.4) becomes significant due to the penalized error, and prompts SMCO to lower reactor pressure to get \(V_{lift}\) off the constraint. Note that the steady-state gain of \(V_{lift}\) with respect to \(P_4^{set}\) is larger than the other two manipulated variables. The SMCO thus lowers the pressure setpoint to offset the increase in lift air blower speed. It can be also seen that there is no negative impact on cost by reduction of \(P_4\), as the cost partials for \(P_4\) are zero (Table 4.4).

However the second step by SMCO towards optimum is smaller, essentially because the error terms in Eq. (4.3) are larger as the constrained variables \(V_{lift}\) and \(V_{11}\) are more nearer to their upper constraints (Figure 4.2e and 4.2f). Lift air blower governor operating point with an upper constraint of 0.65 is the principal error in this case which dominates the optimization (Figure 4.2e). SMCO slowly drives the FCC unit towards an optimum. The wet gas suction valve, \(V_{11}\) with an upper constraint of 0.95 (Figure 4.2f) and the lift air blower compressor capacity are the two constrained variables which limit the further optimization of the FCC unit. The reactor temperature reaches its upper constraint of 995°F and is maintained there throughout the operation (Figure 4.3c). The lowering of the reactor pressure (Figure 4.3b) is limited by the constraint on the manipulated variable for the pressure controller \((V_{11})\) which has an upper constraint of 0.95. Higher feed rates and higher reactor temperatures result in increased production of gasoline and lighter gas (Figure 4.3e and 4.3f). This adds to the revenue as reflected in the lower costs (Figure 4.3h). Note, that according the formulation of Eq. (4.7), negative cost means profit. The SMCO is successful in driving down the cost by up to $6000/day. Table 4.7 shows the synopsis of the results obtained by application of SMCO to the FCC process.
Another interesting dynamics is seen here in the regenerator temperature. The regenerator temperature reduces in the beginning (Figure 4.2c) because higher amounts of hot regenerated catalyst are required to increase the reactor temperature and the catalyst inventory in the regenerator is reduced, (Figure 4.3d). Also the gas-oil feed is increased meaning more hot catalyst is required and less heat is brought back to the regenerator. This reduces the regenerator temperatures. However the effect is short-lived and the regenerator temperature starts to increase again as increased amounts of coke starts coming in the regenerator because of increased gas-oil feed to the reactor. However further reduced catalyst inventory and constraints on air blower capacities reduce the regenerator temperatures a little more before an optimal steady state is achieved.

Table 4.8: FCCU On-line Optimization: Optimum Conditions, Optimal State

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_{sp}$</td>
<td>14.1 ft</td>
</tr>
<tr>
<td>$T_{diff}$</td>
<td>13.60 °F</td>
</tr>
<tr>
<td>$T_{reg}$</td>
<td>1274.9°F</td>
</tr>
<tr>
<td>$P_0$</td>
<td>29.4 psig</td>
</tr>
<tr>
<td>$V_{lift}$</td>
<td>0.61</td>
</tr>
<tr>
<td>$V_{11}$</td>
<td>0.93</td>
</tr>
<tr>
<td>$T_{feed}$</td>
<td>460.9 °F</td>
</tr>
<tr>
<td>$T_{amb}$</td>
<td>75 °F</td>
</tr>
<tr>
<td>$\psi$</td>
<td>1.00</td>
</tr>
<tr>
<td>AC-1 set</td>
<td>300 ppm</td>
</tr>
<tr>
<td>FC-1 set</td>
<td>81.21 lb/s</td>
</tr>
<tr>
<td>TC-1 set</td>
<td>995.0 °F</td>
</tr>
<tr>
<td>dPC-1 set</td>
<td>-3.56 psig</td>
</tr>
<tr>
<td>TC-2 set</td>
<td>1276.5 °F</td>
</tr>
<tr>
<td>FC-2 set</td>
<td>124.6 lb/s</td>
</tr>
<tr>
<td>PC-1 set</td>
<td>32.94 psia</td>
</tr>
</tbody>
</table>

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Figure 4.2: SMCO application to Model IV FCC unit - I
Figure 4.3: SMCO application to Model IV FCC unit - II

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4.5.2 Disturbances

Three primary disturbances are implemented to test the ability of SMCO in handling the disturbances. The disturbances are: unmeasured feed composition changes, ambient temperature disturbance and feed temperature change. Since feed composition is not modeled in detail, a feed composition change is simulated by altering a single factor which governs the coke yield \( \psi_f \). The initial state for all the disturbances testing, is the optimal state described in the preceding section. Table 4.8 gives the initial conditions for all the runs described hereafter, with SMCO in on mode.

Feed Composition Disturbance

The coking characteristics of various feeds is parameterized by a single factor \( \psi_f \). McFarlane et al (1993) describe it as:

\[
\psi_f = \begin{cases} 
1 & \text{normal gas oil} \\
> 1 & \text{heavier than normal gas oil} \\
< 1 & \text{lighter than normal gas oil}
\end{cases}
\]

Figures 4.4 and 4.5 show the responses of the constrained and manipulated variables to disturbances in feed composition change when SMCO is on. A 2.5 % step disturbance in coking factor, \( \psi_f \) is introduced when the SMCO is operating at the optimum setpoints determined in the previous section (Figure 4.5g). The increased \( \psi_f \) results in a rapid increase in coke deposition on the catalyst in the riser and the concentration of coke on spent catalyst (not shown) increases. This additional coke is transported to the regenerator with the spent catalyst, resulting in higher combustion rates in the regenerator and thus a rapid increase in the regenerator temperature (Figure 4.4c).
The COSG controller (AC-1) calls for more air from the lift air blower to maintain the concentration of carbon monoxide at 300 ppm. The lift air blower responds by operating at higher speeds to meet the demand. The constraint of 0.65 on the lift air blower speed is violated. This is acceptable since it is not a very stringent constraint and can be violated to quell the disturbances. In order to bring the $V_{lift}$ back to within its constraint (Figure 4.4e) SMCO reduces the feed flow of gas oil (Figure 4.5a). If the $V_{lift}$ constraint had only been very near to its constraint (without violating it) SMCO would have reduced the feed only. This is observed in presence of ambient temperature disturbance (described in the next section) where $V_{lift}$ approaches very close to its upper constraint but never violates it. In this case the constraint is violated and the control term in Eqn. (4.4) is highly emphasized. Thus SMCO uses all the possible manipulated variables to get the variable within its constraints disregarding the optimization task. Thus it lowers reactor temperature simultaneously (Figure 4.5c). It also reduces the reactor pressure $P_4$ (Figure 4.5b) because as seen from Table 4.3 the reactor pressure has a larger gain than $T_r$ or $F_2$ for $V_{lift}$. Once the $V_{lift}$ is within its bounds the gas oil and reactor temperature are increased again for maximum profits and reactor pressure is driven down further.

An opposite behavior is observed when a negative step in $\psi_f$ is introduced. Thus it can be seen that SMCO handles the unmeasured feed disturbances very well and tracks the new optimum without violating any constraints.

**Ambient Temperature Disturbance**

Figures 4.6 and 4.7 show the responses of the constrained and manipulated variables to ambient temperature disturbance when SMCO is on. Ambient temperature disturbance is simulated as a sinusoidal change in the ambient temperature over a 24 hour period as seen in Figure 4.7(g). As ambient temperature increases, the air blower throughput is
Figure 4.4: SMCO application to Model IV FCC unit in presence of feed composition disturbance - I

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Figure 4.5: SMCO application to Model IV FCC unit in presence of feed composition disturbance - II
known to decrease. Lower blower throughput causes the excess oxygen concentration in the regenerator to decrease. This increases the carbon monoxide concentration in the stack gas. The COSG controller (AC-1) calls for more air from the lift air blower. The lift air blower supplies more air to the regenerator by increasing the speed but this causes the \(V_{\text{lift}}\) to be very near to its upper constraint. This is acceptable since it is not a stringent constraint and can be violated to quell short-term disturbances. To bring the \(V_{\text{lift}}\) back within its constraints, the SMCO has to either lower the reactor pressure or lower the feed rate to the reactor. Note: The steady state gain (Table 4.3) for \(P_1^{\text{set}}\) is larger than \(F_1^{\text{set}}\). It is not possible to lower the reactor pressure further because the manipulated variable \((V_{11})\) of the reactor pressure controller (PC-1) is already near its constraint. The SMCO thus lowers the feed rate to bring back the \(V_{\text{lift}}\) within its constraints. Figure 4.7(a) shows that SMCO drives down the feed rate and the \(V_{\text{lift}}\) is brought back within its constraint. When the feed rate to the reactor is reduced, less amount of catalyst is required by the reactor. The extra hot catalyst is retained in the regenerator which in turn increases the regenerator temperature slightly (Figure 4.6c). When the ambient temperature is on a decline during the night time, the capacity of the air blower increases and more feed can be processed by the unit. Thus SMCO increases the feed rate of gas-oil (Figure 4.7a) beyond its optimal value at no disturbance. The extra revenue is reflected in the cost plot (Figure 4.7h) as extra profits. If the FCCU was to be operated without SMCO, the unit would have to be operated at the feed rate suitable at the highest ambient temperature. This would have resulted in the loss of revenue of $1000/day. The increased production rate increases the pressure in the reactor as seen in Figure 4.7(b). This is acceptable as the wet gas suction valve is within its constraints.
Figure 4.6: SMCO application to Model IV FCC unit in presence of ambient temperature disturbance - I
Figure 4.7: SMCO application to Model IV FCC unit in presence of ambient temperature disturbance - II
Feed Temperature Disturbance

Figures 4.8 and 4.9 show the responses of the constrained and manipulated variables to feed temperature disturbance when SMCO is on. A feed temperature disturbance is simulated as a positive and a negative step change when the process is operating at its optimal state as described in section 4.5. As seen in Figure 4.9(g) a negative step change of 10 °F is made in the feed inlet temperature. This in turn suddenly drops the reactor temperature (Figure 4.9c). The reactor temperature controller (TC-1) increases the differential pressure thus increasing the flow of catalyst to the reactor. This has the effect of increasing coke production in the riser. The reduction in inventory of hot catalyst in the regenerator (Figure 4.9d) briefly lowers the regenerator temperatures (Figure 4.8c) and hence the combustion rates in the regenerator. However additional coke from the reactor is transported back to the regenerator which is burnt off and this increases the regenerator temperature. This increases the carbon monoxide concentration in the stack gas. To maintain the COSG controller setpoint, the speed of the lift air blower increases and violates the constraint of 0.65 (Figure 4.8e). This is again acceptable as additional air can be supplied to avoid violating the more important constraint of COSG (≤ 350 ppm). To bring the $V_{lift}$ back within its constraint, SMCO reduces feed and reactor temperature setpoint simultaneously (Figure 4.8a and 4.8c) for the reasons explained in the feed composition disturbance section. Once the $V_{lift}$ is back within its constraints, the reactor temperature is increased back again. The feed is decreased in small quantities further because $V_{lift}$ is still not at its previous value and is close to the constraint upper limit of 0.65. When the feed temperature is brought back to its original value, it increases the reactor temperature slightly causing a momentary increase in the coke production which is transported to the regenerator. The additional carbon spike causes the carbon
Figure 4.8: SMCO application to Model IV FCC unit in presence of feed temperature disturbance - I
Figure 4.9: SMCO application to Model IV FCC unit in presence of feed temperature disturbance - II
monoxide concentration to rise. The AC-1 quells this disturbance by increasing the air flow rate setpoint. FC-1 complies by increasing $V_{lift}$. During these events, SMCO samples the process and sees that the $V_{lift}$ constraint is violated. It thus reduces the feed rate to the reactor and the reactor temperature again to bring back the $V_{lift}$ back within its limits. At the next sample time of SMCO, the $V_{lift}$ is within its constraint and thus feed rate and the reactor temperature are again increased.

When a positive step disturbance is introduced in the feed temperature similar behavior is observed in the reverse direction. Additional feed can be processed and the production rate can be increased. SMCO increases the feed rate up to a point by which the lift air blower operates near its constraint of 0.65. The wet gas suction valve is seen switching because it opens when the reactor pressure setpoint is lowered while it closes when the feed to the reactor is decreased (as less product gases are formed and the valve has to close to maintain the pressure setpoint).

4.6 Valve Position Control Strategy (VPCS)

Linares (1994) proposed a control scheme for the Amoco model described in chapter 3. He used two valve position controllers in the control scheme which was similar to the one described in section 3.6. In the scheme (as shown in Figure 4.10) the COSG controller was cascaded with a flow controller which manipulates the combustion air blower suction valve ($V_b$) instead of the lift air blower speed. A valve position controller was employed which holds the valve ($V_b$) at 95% open position all the time. The valve position controller (VPC-1) manipulates the setpoint of the reactor pressure controller (PC-1) to maintain the valve at its desired position. Similarly, another valve position controller (VPC-2) was employed to maintain the wet-gas compressor suction valve ($V_{i1}$) at the position of
95% open. This valve position controller (VPC-2) manipulates the setpoint of feed flow controller (FC-2) to maintain the $V_{11}$ valve at its desired position.

For comparing VPCS with SMCO, two similar valve position controllers are employed however COSG controller (AC-1) is cascaded with the flow controller (FC-1) which manipulates lift air blower speed ($V_{lift}$). This is done to keep the regulatory control scheme same for VPCS and SMCO. Figures 4.11 and 4.12 show the response of FCCU to valve position control strategy (VPCS). As seen from figure (4.12a) the feed to the reactor is increased rapidly until the $V_{11}$ valve is at its setpoint of 95% open. Valve position

Figure 4.10: Valve position control scheme for FCCU, (Linares, 1994)
controller (VPC-2) increases the setpoint of the feed flow controller to bring the valve to its nominal operating point of 95% open. Similarly the VPC-1 reduces the pressure controller setpoint (PC-1) to bring the \( V_{liq} \) to its operating point of 0.65. This control strategy showed an equivalent performance to the on-line optimization of the FCC unit using SMCO as described before. It also handled the benchmark disturbances very well. However the method proves to be an effective on-line optimization tool in this case for one reason only - The optimal setpoints lie at the constraint boundaries. For example, the optimal reactor temperature is at its upper constraint of 995 °F. The valve position control strategy cannot increase or decrease the reactor temperature setpoint like SMCO and thus if the VPCS was applied to the FCCU at the base case (at initial conditions shown in Table 4.6) described before, the reactor temperature would have been held constant at 991 °F, and the SMCO would have proved superior. The limiting constraints which limit the further optimization of the unit, using SMCO, are lift air blower speed (\( V_{liq} \)) and wet gas compressor suction valve (\( V_{j1} \)). Both of which saturate to their upper constraints. If the optimal setpoints were to lie in the region somewhere between the upper and lower limit of the limiting constraints, the valve position control strategy will not be useful. The valve position control strategy would then try and drive the process to its constraints irrespective of the optimal setpoints. Also any change in the process gains would require the valve position controllers to be retuned. Chapter 5.4 demonstrates the on-line optimization of a CSTR where the optimum does not lie at the constraint boundaries but somewhere in between. Valve position control strategy won't be able to track that optimum.

4.7 Summary

In this chapter the SMCO algorithm by Daniel et al (1994) was applied to a Model IV FCC unit. The SMCO was found to have successfully optimized the process within...
the operating constraints. The details of implementation were given regarding the cost-function formulation, the constrained and manipulated variables identification, the cost partials and the steady-state gain matrix which acts as the steady-state model of the process. Benchmark disturbances of feed composition, feed temperature and ambient temperature were simulated and it was shown that SMCO handles the disturbances very well and tracks the drifted optimum caused by the disturbances. Valve position control strategy (VPCS) by Linares, 1994 was described and the performance was compared with the on-line optimization of FCCU, using SMCO. It was found that VPCS can prove beneficial, only if the optimal setpoints lie at the constraints, and do not change with changing operating conditions, over time.

Next chapter proposes an on-line steady-state gain identification (OSGI) method which is useful in tracking drifted steady-state gains. The method finds its application in multi-variable control and on-line optimization which use steady-state gains.
Figure 4.11: Valve Position Control Strategy for FCCU - I
Figure 4.12: Valve Position Control Strategy for FCCU - II
Chapter 5

On-line Steady-state Gain Identification

5.1 Introduction

A difficult task of the multi-variable control system is identification of the process gain matrix. The steady state gain matrix (SSGM) is usually constructed by perturbing manipulated variables to get the responses of the controlled variables. The usual way to identify the gains of a process is to introduce perturbations into the process manipulators and to measure the final resulting changes in the process outputs with control loops opened. This approach is usually referred to as open-loop identification.

Theoretically the steady-state-gain-matrix is valid only about a particular state of process at which the data are collected. The control system relying on this SSGM deteriorates when the process gains deviate from those represented by the constant matrix. When this occurs a new SSGM has to be estimated. Deterioration is gradual and partial because in many cases, only some of the elements, of the matrix are changed. One of the difficulties is to determine when a new matrix is needed (Lin, 1993).

Papastathopoulou and Luyben (1990) demonstrated a new method for the derivation of steady-state gains using small perturbations in the set-points instead of the manipulated variables. The identification is made in closed loop running the system under feedback control with integral action in the controllers and making a change in the set-point of one of the controlled variables. The resulting final changes in the manipulated variables are then measured and the corresponding gains are calculated. This is termed as closed-loop identification. McIntosh and Mahalec (1991) showed the use of a similar method.
to calculate steady-state gains using 'swings'. However, the steady-state gains can be derived only off-line using these methods.

This chapter presents an On-line Steady-state Gain Identification (OSGI) method which is similar to the gradient algorithm by Goodwin et al (1980). The gradient algorithm uses the past input and output values every sample whereas the OSGI algorithm uses only the current steady state sample values of the inputs and outputs. The method identifies a new SSGM using estimates from the previous sample. The method is essentially applicable to track the drifting SSGM caused by changes in the operating conditions over time. The application of the method is demonstrated on a simple binary distillation example.

5.2 Proposed Method

The SSGM is represented as matrix $A$ with elements $a_{ij}$ where $i$ represents $i^{th}$ controlled variable and $j$ represents the $j^{th}$ manipulated variable. In other words:

$$a_{ij} = \frac{\Delta y_i}{\Delta u_j}$$

(5.1)

Thus if steady state gains are correct the change in controlled variable can be predicted using equation (5.1):

$$\Delta y_i = \sum_{j=1}^{m} a_{ij}\Delta u_j \quad for \ i = 1, \ldots, n$$

(5.2)

In vector-matrix form:

$$\Delta \mathbf{y} = A \Delta \mathbf{u}$$

(5.3)
The prediction error is defined as the difference between the actual output and the predicted output.

\[ e(k) = \Delta y(k) - \Delta \hat{y}(k) \]
\[ = \Delta y(k) - A(k - 1)\Delta u(k) \quad (5.4) \]

where,

\[ \Delta y(k) = y(k) - y(k - 1) \quad (5.5) \]

and

\[ \Delta u(k) = u(k) - u(k - 1) \quad (5.6) \]

and \( k \) is the steady-state sample. The steady state gain matrix will be representative only when the prediction error between the actual output and the predicted output is minimum. Thus an algorithm similar to gradient algorithm (Goodwin et al., 1980) for steady state samples (for a MIMO model) can be given as:

\[ \hat{\theta}_i(k) = \hat{\theta}_i(k - 1) + \frac{[y_i(k) - \hat{\theta}_i^T(k - 1)\Delta u(k)]\Delta u^T(k)}{\lambda + \Delta u(k)^T\Delta u(k)} \quad (5.7) \]

where,

\[ \hat{\theta}_i = [a_{i1} \ a_{i2} \ \ldots \ a_{im}]^T \]

and

\[ \Delta u = [\Delta u_1 \ \Delta u_2 \ \ldots \ \Delta u_n]^T \]

Taking advantage of the common denominator in Eqn. (5.7), it can be expressed in a vector-matrix form as:
\[ A_k = A_{k-1} + \frac{e_k \Delta u_k^T}{\lambda + \Delta u_k^T \Delta u_k} \]  

(5.8)

where,

\[ A = [\theta_1^T \theta_2^T \ldots \theta_m^T]^T \]

and where \( \lambda \) is the move suppression parameter which determines the speed of convergence. Note that the product \( \Delta u^T \Delta u \) is a scalar.

The convergence properties of the gradient algorithm were studied using a Lyapunov-type analysis, by Goodwin et al. (1980). The complete proof of convergence is given in Goodwin and Sin (1984). The OSGI algorithm is similar to the gradient algorithm except for the fact that it uses only current steady state samples.

### 5.2.1 Perturbation Signal

An external signal (a perturbation signal) must be provided for the method to converge to reasonable estimates of SSGM. The popular perturbation signal is the PRBS (pseudo random binary sequence). The period of a PRBS signal should be longer than the significant duration of the process impulse response (Eveligh, 1967). At each sampling interval the PRBS is added to the process input. In the closed loop the PRBS may be added either directly to the controller output, which is the process input, or to the set-point. The sampling interval must be at least as long as the time it takes for the slowest output of the process to reach a steady-state.

The use of PRBS as a perturbation signal has an advantage that the set-points change asynchronously and thus can estimate the individual effect of each input on the system. This helps in the quick estimation of the steady-state gains.
5.2.2 Startup

The OSGI method works well if reasonable estimates are provided at the startup of the method. The start-up SSGM can be determined by open-loop identification, through a priori knowledge about the transfer function matrix of the system or through some other suitable method. This method is essentially designed to track the changing steady-state-gain-matrix as the process moves from one steady state to another, either due to disturbances or due to some moves (like in optimization) of the process input.

5.2.3 Move Suppression Parameter

The move suppression parameter $\lambda$ determines the amount of change possible in the SSGM in order to reduce the prediction error. Larger values of $\lambda$ slow down the speed of convergence while very small values can cause the estimates to overshoot.

5.2.4 Algorithm

Consider the 2 x 2 system as shown in fig. 5.1. As seen in the figure, $y_1$ and $y_2$ are the controlled process outputs while $u_1$ and $u_2$ are the inputs to the process. The PRBS signal is added as the set-point to the two feedback controllers which in turn will perturb the system around its initial steady state.

The steady state gain matrix of the system relating controlled and manipulated variables in terms of deviation variables is:

$$
\begin{bmatrix}
\Delta \hat{y}_1 \\
\Delta \hat{y}_2
\end{bmatrix} =
\begin{bmatrix}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{bmatrix}
\begin{bmatrix}
\Delta u_1 \\
\Delta u_2
\end{bmatrix}
$$

(5.9)

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Figure 5.1: Schematic for Wood & Berry binary distillation

The PRBS signal is added to the set-points of the two controllers, as shown in fig. 5.1, at every steady state sample. Thus $u_1$ and $u_2$ will change to achieve the desired set-points. Then at every sample interval of OSGI the following steps are carried out:

1. Calculate $\Delta y$ and $\Delta u$ using equations (5.5) and (5.6) respectively.

2. Calculate $e_k$ using equation (5.4).

3. Apply equation (5.8) with some pre-determined value of $\lambda$. 

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The algorithm is started with an initial start-up estimate of the steady-state-gain-matrix £\( A \), which can be determined by open-loop identification or through a priori knowledge about the transfer function matrix of the system. Since this method is designed essentially to track the drifting SSGM, initial estimates are assumed to be known.
5.2.5 Example

Consider the binary distillation example first reported by Wood and Berry (1973)

\[
G(s) = \begin{bmatrix}
12.8e^{-4} & -18.9e^{-3s} \\
16.7s+1 & 21.0s+1 \\
6.6e^{-1s} & -19.4e^{-3s} \\
10.9s+1 & 14.4s+1
\end{bmatrix}
\] (5.10)

The SSGM for the system is:

\[
A = G(0) = \begin{bmatrix}
12.8 & -18.9 \\
6.6 & -19.4
\end{bmatrix}
\] (5.11)

Let's assume that due to some disturbances or changes in the operating conditions the SSGM drifts to the steady state gains of:

\[
A = \begin{bmatrix}
10.0 & -16.0 \\
8.0 & -22.0
\end{bmatrix}
\] (5.12)

Note from Figure 5.1 the perturbations are introduced in the controlled variables \(y_i\). The controllers then try and achieve the setpoint given by the PRBS. In doing so the manipulated variables deviate from their original value. This change in manipulated variables \(u_j\) is measured. This is exactly opposite of what is done in open-loop identification where, manipulated variables are perturbed and the change in process outputs is recorded. Mathematically it can be viewed as:

\[
\Delta u = A^{-1}\Delta y = A'\Delta y
\] (5.13)
Thus $A' = A^{-1}$ is given as the initial SSGM to the OSGI algorithm. As suggested by Papastathopoulou and Luyben (1990), for closed-loop identifications, the inverse of the SSGM ($A^{-1}$) is estimated and then inverted back to get the SSGM. The PRBS signal is added as shown in fig. 5.1. Fig. 5.2 shows the dynamic response of the system to the PRBS signal. The sample interval for OSGI is 100 s which is long enough to achieve steady-state for both $y_1$ and $y_2$. The controllers which implement the set-points were tuned from Luyben (1986), based on initial steady-state gains. Thus at every sample $\Delta y_1, \Delta y_2, \Delta u_1$ and $\Delta u_2$ values are calculated using equations (5.5) and (5.6) and a new SSGM is estimated using equation (5.8).

The OSGI at the end of 10 samples estimated the gains as:

$$
\hat{A}^{-1} = \begin{bmatrix}
0.2361 & -0.1767 \\
0.0870 & -0.1113
\end{bmatrix}
$$

(5.14)

which on inverting gives the estimated SSGM as:

$$
\hat{A} = \begin{bmatrix}
10.21 & -16.21 \\
7.98 & -21.66
\end{bmatrix}
$$

(5.15)

The prediction of the SSGM as shown in this equation is reasonably close to the actual SSGM in equation (5.12).

### 5.3 Discussion

The sampling interval of OSGI is critical. It is necessary that the sampling interval be greater than or equal to the time required by all the process outputs to attain a steady-state. Since OSGI is essentially designed to work on steady-state data, unsteady state data will force the algorithm to predict unrealistic results.
The OSGI does not have to be run continuously on-line, but could be switched on for a period of time only, when the SSGM is suspected to have changed. A perturbation signal is desirable in order to achieve convergence. The perturbation signal should be large enough so that it is not masked by noise or unmeasured disturbances. To ensure that only steady-state data is used in identification, the SSGM may not be updated when unmeasured disturbances enter the system. The steady-state can be detected (as shown in Figure 5.3) by taking standard deviation of say 10 point moving average. The process can be assumed to be at a steady-state when the standard deviation of moving average is less than some predetermined tolerance (Oliver Smith, 1996). If the standard deviation is larger, the data could be ignored and the SSGM is not updated.

- Use Standard Deviation of 10 point Moving Average
- Steady State when S.D. < \( \varepsilon \)

![Figure 5.3: Steady-State Detection (from Smith, 1996)](image)

5.4 Summary

A steady-state-gain-matrix estimator method is proposed. This method is applied on-line to the steady state data with a reasonable initial estimate. It can converge to the true gains
fairly quickly and is easy to program on any digital computer. It is essentially useful in tracking the drifting SSGM caused by changes in operating conditions over time. The application of the method is demonstrated on a simple binary distillation example. The method finds its application more suitable to on-line optimization as shown in next chapter.
Chapter 6
Application of OSGI and SMCO to a CSTR

6.1 Introduction

To demonstrate the application of On-line Steady-state Gain Identification (OSGI) in on-line optimization it is applied to a continuously stirred tank reactor (CSTR) in combination with Supervisory Multivariable Constrained Optimization (SMCO). OSGI essentially helps in identifying the process model and the cost partials in the SMCO at every new steady-state and thus makes SMCO effective over a wider range of operation. Two kinds of reactions are considered: irreversible and reversible. The method shows its efficacy more in the reversible case where the optimum shifts appreciably with changing operating conditions, and needs to be tracked down.

6.2 Irreversible Reaction

Consider a CSTR as shown in Figure 6.1 where a simple irreversible exothermic reaction takes place:

\[ A \rightarrow B \]

The above CSTR with coolant dynamics was reported by Bartusiak et al (1989) and the differential equations which describe the model are as follows:

\[
\frac{dC_A}{dt} = \frac{q}{V} (C_{Af} - C_A) - k_0 e^{-E/RT_c} C_A \tag{6.1}
\]

\[
\frac{dT_r}{dt} = \frac{q}{V} (T_f - T_r) + \frac{(-\Delta H)}{\rho C_p} k_0 C_A e^{-E/RT_c} + \frac{UA}{\rho C_p V} (T_c - T_r) \tag{6.2}
\]
Figure 6.1: Schematic of CSTR: Reversible Reaction

\[
\frac{dT_c}{dt} = \frac{q_c}{V_c} (T_{cf} - T_c) + \frac{UA}{\rho_cC_pV_c} (T_r - T_c)
\]  

(6.3)

which has the steady-state values and physical properties shown in Table 6.1. As described

Table 6.1: Steady-state operating conditions and properties for CSTR: irreversible reaction

<table>
<thead>
<tr>
<th>(V)</th>
<th>100 lit</th>
<th>(C_p)</th>
<th>0.239 J/gm K</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V_c)</td>
<td>40 lit</td>
<td>(C_{pe})</td>
<td>0.239 J/gm K</td>
</tr>
<tr>
<td>(UA)</td>
<td>50,000 J/min °K</td>
<td>(T_f)</td>
<td>323 °K</td>
</tr>
<tr>
<td>(k_0)</td>
<td>(7.2 \times 10^{10}) min(^{-1})</td>
<td>(T_{cf})</td>
<td>287 °K</td>
</tr>
<tr>
<td>(E/R)</td>
<td>8750 °K</td>
<td>(q_c)</td>
<td>100 lit/min</td>
</tr>
<tr>
<td>(-\Delta H)</td>
<td>50,000 J/mol</td>
<td>134.8 lit/min</td>
<td></td>
</tr>
<tr>
<td>(\rho)</td>
<td>1000 gm/lit</td>
<td>(C_{Af})</td>
<td>1.0 mol/lit</td>
</tr>
<tr>
<td>(\rho_c)</td>
<td>1000 gm/lit</td>
<td>(T_r)</td>
<td>420.0 °K</td>
</tr>
<tr>
<td>(C_A)</td>
<td>0.0153 mol/lit</td>
<td>(T_c)</td>
<td>367.9 °K</td>
</tr>
</tbody>
</table>

in Chapter 4 SMCO requires that constrained and manipulated variables for the application be determined and that a cost-function be formulated. A steady-state gain matrix has to
be formed which serves as the process model. The minimum and the maximum limits on the constrained variables have to be determined.

### 6.2.1 Constrained and Manipulated Variables

The coolant flow rate is the manipulated variable of the lower level regulatory controller. A finite flow rate of coolant is possible because of the practical constraints on either the pump or the valve supplying the coolant. To account for these constraints, the coolant flow rate is decided as the constrained variable for the SMCO. The upper limit on the coolant flow is the maximum possible flow, through the valve. The lower limit can be fixed arbitrarily. The upper limit on the coolant flow rate is fixed such that the SMCO doesn’t push the CSTR to an operating state where maximum possible coolant flow is forced, and no safety margin is left to respond to temperature disturbances. The lower level regulatory controller should have some margin of safety to quell any short-term disturbances and maintain the temperature of the reactor at the desired level. The manipulated variables for SMCO are the feed flow rate setpoint and the reactor temperature setpoint. Table 6.2 gives the upper and lower limits on the constrained variables and the manipulated variables. The constraints on the manipulated variables ($T_r^{set}$ & $q^{set}$) are referred to as hard constraints because the manipulated variables are adjusted by the algorithm and their constraints can be directly enforced. On the other hand, dependent variable constraints ($q_c$) are really just soft boundaries that can only be enforced through the adjustments of the manipulated variables. The SSGM is formed as described in section 4.3, by step-testing each manipulated variable, while holding other manipulated variables constant. The SSGM formed is shown in Table 6.3. These gains are changes in the flow rate of coolant per unit change in each of the manipulated variables. For example, the gain $\frac{\partial q_c}{\partial T_r^{set}} = -2.60$ lit/min per °K is the resulting change in the coolant flow rate per unit
Table 6.2: Constrained and Manipulated Variables for CSTR: irreversible reaction

<table>
<thead>
<tr>
<th></th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coolant flow rate, lit/min</td>
<td>110 $q_c$</td>
<td>190</td>
</tr>
<tr>
<td>Reactor Temperature setpoint, °K</td>
<td>378 $T_{set}$</td>
<td>500</td>
</tr>
<tr>
<td>Reactor Feed rate setpoint, lit/min</td>
<td>50 $q_{set}$</td>
<td>150</td>
</tr>
</tbody>
</table>

Table 6.3: SSGM for CSTR: irreversible reaction

<table>
<thead>
<tr>
<th></th>
<th>$T_{set}$</th>
<th>$q_{set}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q_c$</td>
<td>-2.60</td>
<td>1.51</td>
</tr>
</tbody>
</table>

increase in reactor temperature. Similarly, the other gain is the change in the coolant flow rate which results from a unit increase in the feed flow rate. The gains presented here were obtained from step tests on the steady-state simulation of the reactor system.

6.2.2 Cost Function

The cost function is formulated as described in Chapter 4. The cost of utilities (e.g. steam, coolant) is neglected. The unused reactants are assumed to be fully recovered and thus have a product value.

$$ C = qC_A V_A - qC_B V_B - qC_A V_A $$

where, unit values of A ($V_A$) and B ($V_B$) are given as $0.45$/mol and $0.5$/mol respectively. SMCO requires cost partials of above equation with respect to manipulated variables. Differentiating the above equation with respect to each manipulated variable, the cost
partials are:

\[ \frac{\partial C_A}{\partial T^\text{set}} = q^\text{set} \frac{\partial C_A}{\partial T^\text{set}} (V_B - V_A) \]  

(6.5)

\[ \frac{\partial C_A}{\partial q^\text{set}} = \left[ q^\text{set} \frac{\partial C_A}{\partial q^\text{set}} + C_A - C_A^f \right] (V_B - V_A) \]  

(6.6)

As seen from the equations above, \( \frac{\partial C_A}{\partial T^\text{set}} \) and \( \frac{\partial C_A}{\partial q^\text{set}} \) are needed to calculate the cost partials with respect to the manipulated variables. The values are given in Table 6.4. These gains are changes in the concentration of reactant A per unit change in each of the manipulated variables. For example, the gain \( \frac{\partial C_A}{\partial T^\text{set}} = -4.75 \times 10^{-4} \text{ mol/°K} \) is the resulting change in the reactant concentration per unit increase in reactor temperature. The gains presented here were obtained from step tests on the steady-state simulation of the reactor system.

Table 6.4: Cost partials for SMCO application to CSTR: Irreversible Reaction

<table>
<thead>
<tr>
<th>( \frac{\partial T^\text{set}}{\partial q^\text{set}} )</th>
<th>( \frac{\partial q^\text{set}}{\partial q^\text{set}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{\partial C_A}{\partial T^\text{set}} )</td>
<td>( -4.75 \times 10^{-4} )</td>
</tr>
<tr>
<td>( \frac{\partial q^\text{set}}{\partial q^\text{set}} )</td>
<td>( 1.0 \times 10^{-4} )</td>
</tr>
</tbody>
</table>

6.2.3 Low Level Regulatory Controllers

A proportional-integral (PI) controller was tuned and employed as a regulatory controller to control the reactor temperature. The manipulated variable for the reactor temperature controller is the coolant flow rate.

The feed flow controller shown in Figure 6.1 is not actually implemented; the feed flow rate is set to equal to its setpoint instantaneously. This is done to avoid the dynamics of the control loop, which are insignificant for the example.
The setpoints of both the controllers are determined by SMCO at every sampling instance of SMCO.

### 6.2.4 Implementation

The differential equations described above are integrated using fourth order Runge-Kutta method. The \( \lambda \) and the \( w_c \) are decided by off-line testing to be 0.8 and 0.05 respectively. A routine implementing OSGI algorithm described in Chapter 5, is programmed. It takes approximately 10 min for the CSTR system to achieve a steady-state. The SMCO sample time is thus set to be 10 min. The OSGI is implemented every 60 min. The period of the pseudo random binary signal (PRBS) described in Chapter 5 is the same as SMCO sample time of 10 min. SMCO is switched off when perturbations are introduced into the system by OSGI. Thus the system alternates between SMCO and OSGI. Both are never switched on at the same time.

### 6.2.5 SMCO Application

As described in Chapter 4, the SMCO is applied to this system. Figure 6.2 shows the response of the system to the on-line optimization by SMCO. The initial conditions for the system are as given in Table 6.1. The feed flow rate and the reactor temperature are increased by SMCO to maximize production rate and thus the profits (Figure 6.2b and 6.2e). The coolant temperature drops initially due to increased flow of the coolant (Figure 6.2c) but starts to increase later as the exothermic reaction with increasing feed, proceeds to produce more heat. However the feed flow rate saturates at its maximum possible value (Figure 6.2e), and from that point onwards SMCO optimizes the process using only one manipulated variable, the reactor temperature keeping the feed flow rate at its saturated value. The reactor temperature is increased, as the cost-partial \( \partial C_A / \partial T_{r_{saturated}} \) is negative.
(meaning an increase in the reactor temperature decreases the reactant concentration and increases the product concentration, see Table 6.4). The coolant flow rate starts dropping to support the demand of increased reactor temperature (Figure 6.2d). The cost keeps on decreasing and approaches a steady-state value (Figure 6.2h). The concentration of reactant A keeps dropping due to increased conversion (Figure 6.2a) at higher temperatures. The SMCO will drive the reactor temperature higher if the cost term weighting factor \(w_c\) is increased.

### 6.2.6 On-line SSGM Identification

At the optimized state, the SSGM (in Table 6.3) is suspected to have changed. An off-line step testing of each manipulated variable as described in section 6.2.1 yields a changed SSGM as shown in Table 6.5.

<table>
<thead>
<tr>
<th>(T^\text{set})</th>
<th>(q^\text{set})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(q_c)</td>
<td>-4.37</td>
</tr>
<tr>
<td>(q_c)</td>
<td>1.89</td>
</tr>
</tbody>
</table>

Table 6.5: SSGM at optimum state, CSTR: Irreversible Reaction

To identify this change in SSGM on-line, OSGI is run alternately with SMCO. The process thus alternates between SMCO (optimization) and OSGI (identification). The SSGM predicted by OSGI at the end of the simulation (reached optimum state) is as shown in Table 6.6.

<table>
<thead>
<tr>
<th>(T^\text{set})</th>
<th>(q^\text{set})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(q_c)</td>
<td>-4.45</td>
</tr>
<tr>
<td>(q_c)</td>
<td>1.85</td>
</tr>
</tbody>
</table>

Table 6.6: SSGM predicted by OSGI at optimum state, CSTR: Irreversible Reaction
Table 6.7: SSGM True and Predicted SSGM at optimum state, CSTR: Irreversible Reaction

<table>
<thead>
<tr>
<th></th>
<th>$T_r^{\text{set}}$</th>
<th>$q_r^{\text{set}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>True</td>
<td>-4.37</td>
<td>1.89</td>
</tr>
<tr>
<td>Predicted</td>
<td>-4.45</td>
<td>1.85</td>
</tr>
</tbody>
</table>

Figure 6.3 shows the SMCO optimization along with OSGI. The initial conditions are the same as shown in Table 6.1. SMCO and OSGI alternate and the drifted SSGM predicted by OSGI, is used by SMCO in the next step. The PRBS signal can be seen as step changes in the manipulated variables (Figure 6.3b and 6.3e).

No appreciable change is seen by applying OSGI to the optimization because the SSGM does not drift appreciably, and the new SSGM does not have any influence in reaching a different optimum. However the OSGI predicts the true gains of the drifted SSGM (Table 6.5) with considerable accuracy (Table 6.7). The gains $\partial C_A/\partial T_r^{\text{set}}$ and $\partial C_A/\partial q_r^{\text{set}}$ in Equations (6.5 and 6.6) are also liable to change and can be predicted by augmenting the SSGM with another row pertaining to $C_A$. The new SSGM will thus look like:

$$
\begin{array}{c|cc}
    & T_r^{\text{set}} & q_r^{\text{set}} \\
\hline
q_c & \partial q_c/\partial T_r^{\text{set}} & \partial q_c/\partial q_r^{\text{set}} \\
C_A & \partial C_A/\partial T_r^{\text{set}} & \partial C_A/\partial q_r^{\text{set}} \\
\end{array}
$$

However the gains do not affect the optimization because they do not undergo any change in sign or do not change significantly in magnitude. The first row of this matrix is used in the optimum move calculation while the entire matrix is used by the OSGI algorithm, to predict the SSGM and the partials of $C_A$ with respect to the manipulated variables.
Figure 6.2: Application of SMCO to CSTR: Irreversible Reaction
Figure 6.3: Application of SMCO and OSGI to CSTR: Irreversible Reaction
Next section shows the application of SMCO and OSGI to a reversible reaction CSTR where optimum temperature drifts at different feed rates.

6.3 Reversible Reaction

Consider the example given by Economou and Morari, (1986) of an ideal continuous stirred tank reactor where the reversible exothermic reaction

\[ A \rightleftharpoons B \]

takes place as shown in Figure 6.4. The coolant dynamics are not included here as in the previous system. A system of coupled ordinary differential equations models the process:

\[
\frac{dC_A}{dt} = \frac{q}{V}(C_{A_f} - C_A) - k_1 C_A + k_{-1} C_B
\]

(6.7)
\[
\frac{dC_B}{dt} = \frac{q}{V}(C_{Bf} - C_B) + k_1 C_A - k_{-1} C_B \tag{6.8}
\]

\[
\frac{dT_r}{dt} = \frac{-\Delta H}{\rho C_p} (k_1 C_A - k_{-1} C_B) + \frac{q}{V} (T_f - T_r) \tag{6.9}
\]

where

\[k_1 = k_{10} e^{-E_1 / RT_r} \quad k_{-1} = k_{-10} e^{-E_{-1} / RT_r}\]

The steady-state operating conditions and physical properties are given in Table 6.8.

Table 6.8: Steady-state operating conditions and properties for CSTR: reversible reaction

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>60 lit</td>
<td></td>
</tr>
<tr>
<td>(k_{10})</td>
<td>5000 1/s</td>
<td></td>
</tr>
<tr>
<td>(k_{-10})</td>
<td>1 \times 10^6</td>
<td></td>
</tr>
<tr>
<td>(E_1)</td>
<td>10,000 cal/mol</td>
<td></td>
</tr>
<tr>
<td>(E_{-1})</td>
<td>15,000 cal/mol</td>
<td></td>
</tr>
<tr>
<td>(R)</td>
<td>1.987 cal/mol °K</td>
<td></td>
</tr>
<tr>
<td>(-\Delta H)</td>
<td>5000 cal/mol</td>
<td></td>
</tr>
<tr>
<td>q</td>
<td>1 lit/sec</td>
<td></td>
</tr>
<tr>
<td>(C_p)</td>
<td>0.239 cal/kg K</td>
<td></td>
</tr>
<tr>
<td>(\rho)</td>
<td>1 kg/lit</td>
<td></td>
</tr>
<tr>
<td>(C_A)</td>
<td>0.4937</td>
<td></td>
</tr>
<tr>
<td>(C_B)</td>
<td>0.5063</td>
<td></td>
</tr>
<tr>
<td>(C_{Af})</td>
<td>1 mol/lit</td>
<td></td>
</tr>
<tr>
<td>(C_{Bf})</td>
<td>0 mol/lit</td>
<td></td>
</tr>
<tr>
<td>(T_r)</td>
<td>431.1 °K</td>
<td></td>
</tr>
<tr>
<td>(T_f)</td>
<td>428.6 °K</td>
<td></td>
</tr>
</tbody>
</table>

The objective is to exemplify the implementation and the potential of the gain identification method for on-line optimization. As seen from fig. 6.5 the reactor equilibrium conversion has a well-defined maximum with respect to reactor temperature. Moreover, the optimum temperature shifts as the feed rate to the reactor changes. The optimization problem is to find the optimal temperature within constraints and with changing feed conditions.
6.3.1 Constrained and Manipulated Variables

As in the section 6.2.1 the constrained and manipulated variables have to be pre-defined for implementing SMCO. Economou and Morari (1986) used inlet feed stream temperature \( T_f \) as the manipulated variable and concentration of B, \( C_B \) as the controlled variable. The inlet feed temperature has an upper and lower constraint and hence is decided as the constrained variable for the SMCO. This will ensure that the reactor is not driven too close to the constraint and enough safety margin is left for the regulatory controller for responding to any short-term disturbances. The manipulated variables are the reactor temperature controller set-point and the feed flow controller set-point. Therefore SSGM is:

\[
\begin{array}{c|cc}
\text{set} & T_f^\text{set} & q^\text{set} \\
\hline
T_f & a_{11} & a_{12} \\
\end{array}
\]

Table 6.9 shows the minimum and maximum limits on the constrained and the manipulated variables. The SSGM is formed initially, as in section 6.2.1, by step testing each
Table 6.9: Constrained and Manipulated Variables for CSTR: reversible reaction

<table>
<thead>
<tr>
<th></th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactor Feed Temperature, lit/min</td>
<td>350</td>
<td>500</td>
</tr>
<tr>
<td>Reactor Temperature, °K</td>
<td>350</td>
<td>500</td>
</tr>
<tr>
<td>Reactor Feed Rate, lit/s</td>
<td>0</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 6.10: SSGM for CSTR: reversible reaction

<table>
<thead>
<tr>
<th></th>
<th>( T_r ) set</th>
<th>( q_{set} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_f )</td>
<td>-1.00</td>
<td>0.05</td>
</tr>
</tbody>
</table>

manipulated variable while keeping all other manipulated variables constant. Table 6.10 shows the SSGM for this system.

6.3.2 Cost Function

The cost function is identical as shown in Eqn. 6.4 with the same assumptions as described before. The unit values of reactant A and product B are also the same. Differentiating the cost function with respect to the manipulated variables yields the equations identical to Eqn. (6.5) and Eqn. (6.6).

Table 6.11 gives the partials of \( C_A \) with respect to the manipulated variables. As described in section 6.2.5 the values were obtained by step-tests on the steady-state simulation of the reactor system with reversible reaction.

Table 6.11: Cost partials for SMCO application to CSTR: Reversible Reaction

<table>
<thead>
<tr>
<th></th>
<th>( \partial T_r ) set</th>
<th>( \partial q_{set} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \partial C_A )</td>
<td>-9.40 ( \times 10^{-4} )</td>
<td>0.1004</td>
</tr>
</tbody>
</table>
6.3.3 Low Level Regulatory Controllers

SMCO operates at a supervisory level in control hierarchy and requires low-level regulatory controllers to implement the optimal set-points it calculates. A non-linear controller using input-output feedback linearization (Henson and Seborg, 1991) is designed and employed, as the lower level controller. The set-point of this non-linear controller is calculated by the SMCO algorithm.

6.3.4 Implementation

The implementation scheme is the same as described for the irreversible reaction CSTR. The λ and ωe values were determined to be 0.5 and 0.6 respectively. OSGI is implemented every 2000 sec while SMCO every 100 seconds. The period of PRBS is same as SMCO.

The $\partial C_A/\partial T^\text{set}_r$ in eqn. (6.5) can be viewed as the gain ($a_{21}$) between the manipulated variable $T^\text{set}_r$ and $C_A$ and $\partial C_A/\partial q^\text{set}$ in eqn. (6.6) as gain ($a_{22}$) between $T^\text{set}_r$ and $C_A$.

Note from fig.6.5 that for a given feed rate, $\partial C_A/\partial T^\text{set}_r$ (slope) changes sign when it crosses the optimum. This in turn changes the sign of the cost-partial in Eqn. (6.5) which would cause the SMCO to drive the reactor temperature in the wrong direction, if the gain is not updated. Thus an on-line identification method is required to predict the magnitude and sign of the slope. OSGI is employed for this purpose.

SMCO (optimization phase) and OSGI (identification phase) are applied alternately, for tracking the drifting optimum, caused by varying operating conditions.

For identification phase, gains pertaining to $C_A$ are appended to the SSGM defined above.

\[
\begin{array}{c|cc}
\hline
& T^\text{set}_r & q^\text{set} \\
\hline
T_f & a_{11} & a_{12} \\
C_A & a_{21} & a_{22} \\
\hline
\end{array}
\]
For the calculation of the optimum moves using SMCO, only the first row of the above matrix is used. For identification using OSGI, the above matrix is used in its entirety. Thus OSGI identifies the drifted SSGM (first row) and the partials of $C_A$ with respect to manipulated variables (second row) at regular intervals as a single matrix.

By applying the (OSGI) equation (5.8), at regular intervals (identification phase) the gains are updated. In the identification phase a pseudo-random binary signal (PRBS) is added to the manipulated variables (reactor temperature set-point and feed flow controller set-point). The gains are initialized at the beginning of the simulation as shown in Table 6.11.

6.3.5 Simulation Results

As seen from fig.6.7 the SMCO increases the reactor temperature set-point at first because $\partial C_A/\partial T_{\text{set}}$ is initialized to a negative value, meaning an increase in reactor temperature decreases the concentration of reactants and increases the concentration of the products. The feed flow rate is held 1 lit/s which is the upper constraint set on the feed flow rate. It can be seen from fig.6.5 that the $\partial C_A/\partial T_{\text{set}}$ undergoes a change in sign at about 435 K. The identification phase, (seen as a PRBS in fig. 6.7 and 6.8), updates the sign and magnitude of the cost partial. This compels the SMCO to drive down the reactor temperature set-point to the desired optimum. The combined effect of SMCO and OSGI hold the reactor temperature very close to its optimum.

Theoretically, the true optimum lies at the point where $\partial C_A/\partial T_{\text{set}}$ is zero. However the combination of SMCO and OSGI hold the reactor temperature quite close to the optimum. After 6 hours the constraint on the feed rate flow is raised to 1.5 lit/s. This prompts the OSGI to identify the new gains in the identification phase. And as explained earlier, the SMCO and OSGI track the drifted optimum and hold the reactor temperature
at the optimum. A second change in the constraint to a lower value of 0.5 lit/s prompts the OSGI to identify a new set of gains and confirms the efficacy of the method. Thus for each feed rate, SMCO combined with OSGI, drive the reactor temperature to its corresponding optimum (as shown in fig. 6.5).

6.4 Summary

The performance of SMCO and OSGI in optimizing a CSTR with irreversible and a CSTR with reversible reaction has been demonstrated. The use of OSGI in re-identifying the gains of SSGM was shown for the irreversible reaction CSTR. The cost partials did not change in sign and hence the optimum did not shift as the operating conditions changed. However it was shown that OSGI can predict the SSGM with reasonable accuracy.

The reversible reaction CSTR has a shift in optimum temperature, when the feed rate to the reactor changes. OSGI coupled with SMCO correctly identified the gains with their changing signs. It was observed that the OSGI and SMCO together hold the reactor at its optimum, at changing feed conditions. SMCO by itself wouldn't have been able to track the drifting optimum by itself, as the gains of the cost partials changed in sign, when the optimum was crossed. The reactor temperature would thus have been continuously increased by SMCO, without the knowledge of the changed sign, of the cost partials.
Figure 6.6: Equilibrium conversion

Figure 6.7: Reactor temperature

Figure 6.8: Feed rate to the reactor
Chapter 7

Conclusions

7.1 Introduction

The preceding chapters presented four results achieved -

- The Amoco model of a Model IV FCC unit was combined with Lee & Groves (1985) model to achieve a product distribution model.

- SMCO algorithm was applied to the FCC process and on-line optimization results were analyzed. On-line optimization was tested in presence of benchmark disturbances to ensure that constraints are not violated.

- An on-line steady-state gain identification method was developed to identify the steady-state gains in a multivariable system.

- To demonstrate the potential of the OSGI method, it was applied in combination with SMCO to a CSTR with an irreversible reaction and with a reversible reaction. It was demonstrated that, the OSGI can track the drifted SSGM and aid SMCO (or any on-line optimization/control method using SSGM) in tracking the drifted optimum.

In this final chapter, a review is done to see what goals have been achieved. The contributions of the OSGI algorithm to the field of multivariable control and on-line optimization are then discussed. Finally, suggestions for future work are given based on issues that arose during the investigation.
7.2 Goals Reached

Supervisory Multivariable Constrained Optimization (SMCO) method was to be applied to a dynamic and nonlinear multivariable process. FCC process model by McFarlane et al (1993) was chosen to test the SMCO. The FCC model was found to be devoid of a product distribution model. To apply on-line optimization more effectively the Lee & Groves model which provides a three lumped product distribution was combined with the Amoco model.

SMCO was successfully applied to this modified Amoco model and the process was shown to be driven to an optimum without violation of any constraints. The objective function was observed to be improved by 3.2%. Benchmark disturbances were introduced in the system and the behavior of SMCO was observed and analyzed. SMCO was found to handle disturbances in a satisfactory fashion. The drifted optimum was found to be successfully followed by SMCO.

An on-line steady-state gain identification (OSGI) method was proposed which identifies the steady-state gain matrix (SSGM) in a recursive manner. The method involves sampling of the process at the steady-state and adaptively modification the gains depending on the error between the actual value and the predicted value. The method is essentially useful in prediction of the drifted SSGM either due to disturbances or due to optimization moves.

The use of OSGI was demonstrated on a simple binary distillation process involving a transfer function matrix. The OSGI was shown to successfully predict the drifted gains. The use of OSGI was further demonstrated in on-line optimization of CSTRs involving irreversible and reversible reactions. The reversible reaction CSTR showed the efficacy of OSGI in tracking drifted optimum.
7.3 Contributions

- Amoco model by McFarlane et al (1993) did not have any yield model to give a product distribution. Lee & Groves model which provides for a yield model was combined with the Amoco model to obtain the product distribution of gasoline, lighter gas and carbon. This enabled to express the cost function more effectively, in terms of products and optimize the unit more realistically.

- A compact and effective identification method was proposed to identify steady-state gains on-line. The use of only steady-state samples of inputs and outputs of the process make the method less computationally intensive. The method identifies the gains in a closed-loop (when the controllers are active) and thus offers minimum offset to the process. The method converges the gains to their true values reasonably fast and is easy to program on any digital computer.

- All steady-state on-line optimization methods require steady-state modeling of the process which invariably involve steady-state gains. The key parameters in the steady-state model have to be recursively identified by a suitable parameter estimation method to account for changing process conditions and environment. This is the most involving step in the on-line optimization of any industrial process. For example - SMCO has a stipulation, that the cost function be expressed in terms of manipulated and/or constrained variables. Also explicit steady-state modeling has to be done using mass and energy balances to express the cost-function in terms of the constrained and manipulated variables. The use of OSGI along with SMCO eliminates the need to have steady-state modeling in order to determine cost partials. The cost-partials with respect to the manipulated variables are simply included as additional rows to the steady-state gain matrix and the new matrix formed, is
identified by OSGI. The original SSGM containing only constrained variables, is used for determining the optimal setpoints.

7.4 Future Work

- The FCCU reactor riser model could be further improved to provide a better product distribution. Recently, a ten lump yield model was reported which could predict the lighter fractions (Riggs, 1996). The main fractionator could be modeled to obtain separated fractions predicted by the riser model. The fractionator could be included in the overall on-line optimization along with the reactor and the regenerator.

- Future work should be performed in further developing the OSGI method. Variation as mentioned in section 2.2.3 should be examined to achieve more accuracy and speed. The method should be also tested on processes which involve a larger number of inputs and outputs and where the steady-state gains change appreciably (example, Tennesse Eastman challenge problem).

- The use of variable move suppression parameter can also be examined in the OSGI. The errors for each predicted output can have very different magnitudes and a single move suppression parameter might prove insufficient. A scaled move suppression parameter can suppress the change, in proportion to the error’s magnitude. The OSGI should also be tested in presence of disturbances. Steady-state detection can be done as described in Chapter 5.

- A field application of the OSGI method as an extension to a steady-state optimization method should be studied. Also the use of the method in optimizing control can be studied.
7.5 Summary

The Amoco model was shown to be enhanced by including a yield model to give a product distribution for the FCC process. The SMCO algorithm was shown to be successfully applied to the process and the process was optimized on-line to reduce the cost of operation. The optimization was studied and analyzed in presence of benchmark disturbances and it was shown that SMCO handled disturbances very well and tracked the drifted optimum effectively.

A new on-line steady-state gain identification method is proposed and tested for identification of steady-state gains in a multivariable distillation control and in on-line optimization of a CSTR involving reversible and irreversible reactions. The method was shown to have more application and efficacy in the processes where the steady-state gains and the optimum drift with varying operating conditions.
Bibliography


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Linares, J. R., *Dynamics and Multivariable Control Scheme for a Model IV Fluid Catalytic Cracking Unit*, MS thesis, Louisiana State University, 1994


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Appendix A

Symbols

- $a_{ij}$: steady state gain between $i^{th}$ controlled variable and $j^{th}$ manipulated variable
- $A$: steady state gain matrix (SSGM)
- $\hat{A}$: predicted steady state gain matrix (SSGM)
- $C$: cost function
- $C_{Af}$: concentration of A in feed, mol/lit
- $C_A$: concentration of A in the reactor, mol/lit
- $C_B$: concentration of B in the reactor, mol/lit
- $C_{O_2,sg}$: Concentration of oxygen in stack gas, mol %
- $e$: error vector between the actual output and the predicted output
- $E$: Error vector for constraints
- $I$: unit matrix
- $k$: steady-state sample interval
- $q$: flow rate of feed, lit/sec
- $T_{amb}$: Ambient temperature, °F
- $T_{cyc}$: Temperature of cyclones, °F
- $T_{feed}$: Temperature of feed, °F
- $u$: vector of manipulated variables
- $u_j$: $j^{th}$ manipulated variable
- $V_A$: value of reactant A, $$/mol
- $V_B$: value of product B, $$/mol
- $W$: Diagonal weight matrix with $w_i$ as diagonal elements
- $w_c$: Weight for cost term
- $w_i$: Weights for constrained variables
- $y$: vector of controlled variables
- $y_i$: $i^{th}$ controlled variable
- $\hat{y}$: prediction vector of controlled variables
- $\hat{y}_i$: prediction of $i^{th}$ controlled variable
- $Y$: Vector of constrained variables
- $Y_{\text{mid}}$: = $(Y_{\text{max}} - Y_{\text{min}})/2$
- $Y_{\text{max}}$: Upper constraint limit vector for $Y$
- $Y_{\text{min}}$: Lower constraint limit vector for $Y$
Superscript

\( set \)  Setpoint of controllers

Greek

\( \Delta \)  change in value from the previous steady-state sample
\( \lambda \)  move-suppression parameter

Diagonal matrix of \( \lambda \)

Miscellaneous

\( \otimes \)  Multiply only the diagonal elements of the first matrix times those in the second;
\( (A \otimes B)_{ij} = A_{ii}B_{jj} \) for \( i=j \),
and \( A_{ij} \) for \( i \neq j \)

Acronyms and Abbreviations

API  American Petroleum Institute
ARMAX  Auto Regressive Moving Average eXogeneous
ARX  Auto Regressive eXogenous
CSTR  Continuous stirred tank reactor
FCC  Fluidized Catalytic Cracking
FCCU  Fluidized Catalytic Cracking Unit
HCO  Heavy Cycle Oil
IV  Instrumental Variable
LCO  Light Cycle Oil
LP  Linear Programming
MAP  Method Approximation Programming
OSGI  On-line Steady-state Gain Identification
RLS  Recursive Least Squares
SMCO  Supervisory Multivariable Constrained Optimization
Appendix B

Amoco Model IV FCCU (McFarlane et al, 1993)

B.1 Feed System

Three fresh feeds are available to the FCCU system; gas-oil from tankage ($F_{go}$), wash oil ($F_1$) and diesel ($F_2$). The sum of these flows is the total fresh feed rate ($F_3$). The slurry recycle ($F_4$) is added to the fresh feed stream after preheating. The model neglects the dynamics of the controllers and the flow streams so the actual flows are equal to the controller setpoints at all times:

\[
\begin{align*}
F_1 &= F_{1}^{\text{set}} \\
F_2 &= F_{2}^{\text{set}} \\
F_3 &= F_{3}^{\text{set}} \\
F_4 &= F_{4}^{\text{set}}
\end{align*}
\]  

(B.1) (B.2) (B.3) (B.4)

B.2 Preheat System

The fresh feed stream ($F_3$) is assumed to enter the preheat furnace at a specified temperature $T_1$ (Note: The preheater is not modeled).

The furnace firebox temperature and the outlet temperature are modeled with the following assumed dynamic energy balances:

\[
\frac{dT_3}{dt} = \frac{1}{\tau_{fb}} \left( F_5 \Delta H_{fu} - UA_f T_{lm} - Q_{loss} \right)
\]

(B.5)

where

\[
T_{lm} = \frac{(T_3 - T_1) - (T_3 - T_2)}{\log \left( \frac{T_3 - T_1}{T_3 - T_2} \right)}
\]

(B.6)

\[
Q_{loss} = a_1 F_2 T_3 - a_2
\]

(B.7)

\[
F_5 = F_5^{\text{set}}
\]

(B.8)

\[
\frac{dT_2}{dt} = \frac{1}{\tau_{fo}} (T_{2,ss} - T_2)
\]

(B.9)

\[
T_{2,ss} = T_1 + \frac{UA_f T_{lm}}{F_3}
\]

(B.10)
B.3 Reactor

The reactor riser is modeled as a dilute phase solid transport line in which hot catalyst from the regeneratr mixes with the feed oil from the preheat system and the recycle oil (slurry) from the main fractionator. A constant coke deposition is assumed.

Coke and wet gas yield models

The yield of coke deposited on the catalyst in the riser is assumed to be affected only by the following: weight hourly space velocity in the riser (WHSV), the concentration of carbon on the regenerated catalyst \((C_{rgc})\), catalyst residence time in the riser \((\tau_r)\) and the coking characteristic of the feeds. The effect of riser temperature is not modeled. Coke production is given by:

\[
F_{\text{coke}} = \frac{1.3557(F_3 + F_4)F_B \tau_r^{-1.9843}}{100 \text{ WHSV}}
\]

where,

\[
\tau_r = \frac{W_{\text{ris}}}{(60F_{\text{rgc}})}
\]

\[
\text{WHSV} = \frac{3600(F_3 + F_4)}{W_{\text{ris}}}
\]

\[
F_B = \frac{\Psi_f F_3 + 3F_4 + 2F_1 - 0.8F_2}{F_3 + F_4}
\]

\[
\Psi_f = 1 \text{ normal gas oil}
\]

\[
> 1 \text{ heavier than normal gas oil}
\]

\[
< 1 \text{ lighter than normal gas oil}
\]

\[
> 0
\]

The yield of wet gas is assumed to be affected only by riser temperature and is given by:

\[
F_{\text{wg}} = (F_3 + F_4) \left[ C_1 + C_2(T_r - T_{\text{ref}}) \right]
\]

Reactor mass balances

Stirred tank dynamics are assumed for the reactor. The coke balance includes the carbon entering the reactor on regenerated catalyst and is given by:

\[
\frac{dC_{sc}}{dt} = \left[ F_{\text{rgc}} C_{rgc} + F_{\text{coke}} - F_{sc} C_{sc} - C_{sc} \frac{dW_r}{dt} \right] \frac{1}{W_r}
\]

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The catalyst balance is given by:

\[
\frac{dW_r}{dt} = F_{rgc} - F_{sc}
\]  

(B.17)

**Reactor riser energy balance**

The riser energy balance also assumes stirred tank dynamics, with negligible heat loss to the surroundings. The heat of cracking is assumed to be simply proportional to riser temperature. The energy balance is written as:

\[
MC_{p_{eff}} \frac{dT_r}{dt} = Q_{in} - Q_{out}
\]  

(B.18)

where,

\[
Q_{in} = Q_{rgc} + F_3c_{p_{sat}}(T_2 - T_{base, f})
\]  

(B.19)

\[
Q_{out} = Q_{cutout} + Q_{slurry} + Q_{cracking} + Q_{ff}
\]  

(B.20)

\[
Q_{cutout} = F_{rgc}c_p(T_r - T_{ref})
\]  

(B.21)

\[
Q_{slurry} = F_4 [c_{p_{sat}}(T_r - T_{ref}) + Q_{sr}]
\]  

(B.22)

\[
Q_{ff} = F_3 [c_{p_{sat}}(T_r - T_{ref}) + Q_{fr}]
\]  

(B.23)

\[
Q_{cracking} = (F_3 + F_4)\Delta H_{crack}
\]  

(B.24)

\[
\Delta H_{crack} = 172.7 + 3(T_r - T_{ref})
\]  

(B.25)

A constant temperature drop across the reactor stripper is assumed:

\[
T_{sc} = T_r - \Delta T_{stripper}
\]  

(B.26)

**Reactor riser pressure balance**

The pressure at the bottom of the reactor riser is needed in the force balance on the regenerated catalyst U-bend. It is given by:

\[
P_{rb} = P_4 + \frac{\rho_{ris} h_{ris}}{144}
\]  

(B.27)

where,

\[
\rho_{ris} = \frac{F_3 + F_4 - F_{rgc}}{v_{ris}}
\]  

(B.28)

\[
v_{ris} = \frac{F_3 + F_4}{\rho_0} + \frac{F_{rgc}}{\rho_{part}}
\]  

(B.29)
The inventory of the catalyst in the riser is needed in the calculation of the catalyst residence time in the riser (Eqn. B.12) and is given by:

\[ W_{\text{ris}} = \frac{F_{\text{rgc}} A_{\text{ris}} h_{\text{ris}}}{v_{\text{ris}}} \]  

(B.30)

**Reactor and main fractionator pressure balance**

The main fractionator is modeled as a single large volume that includes the volume of piping and the intermediate vessels between the main fractionator and the wet gas compressor. It is modeled with assumed dynamics given by:

\[ \frac{dP_5}{dt} = 0.833(F_{\text{wg}} - F_{v11} - F_{v12} + F_{v13}) \]  

(B.31)

where,

\[ F_{v12} = k_{12} V_{12} \sqrt{P_3 - P_{\text{atm}}} \]  

(B.32)

and \( F_{v11} \) and \( F_{v12} \) are given in next section. A constant pressure drop between the main fractionator and the reactor is assumed, giving the reactor pressure as:

\[ P_4 = P_5 + \Delta P_{\text{frac}} \]  

(B.33)

**B.4 Wet gas Compressor**

The wet gas compressor is modeled as a single stage centrifugal compressor driven by a constant-speed electric motor. It is assumed that the compressor is pumping against a constant pressure in the vapor recovery unit. The compressor performance equation relates suction flow to polytropic head. A single surge point is specified.

The performance equation is given by:

\[ F_{\text{sucn,wg}} = 11600 + \sqrt{1.366 \times 10^8 - 0.1057 H_{\text{wg}}^2} \]  

(B.34)

where,

\[ H_{\text{wg}} = 182922.1(C_{\text{ru}}^{0.0942} - 1) \]  

(B.35)

\[ C_{\text{ru}} = \frac{P_{\text{ru}}}{P_7} \]  

(B.36)

The molar flow rate through the compressor is obtained from the ideal gas law:

\[ F_{11} = 2.636 \times 10^{-6} F_{\text{sucn,wg}} P_7 \]  

(B.37)

The pressure balance around the compressor is given by assumed dynamics:

\[ \frac{dP_7}{dt} = 5(F_{v11} - F_{11}) \]  

(B.38)
\[ F_{V_{11}} = k_{11} f_{pp}(V_{12}) \sqrt{P_5 - P_1} \]  \hspace{1cm} (B.39)

\[ F_{V_{13}} = k_{13} V_{13} P_{\text{ru}} \]  \hspace{1cm} (B.40)

Certain valve characteristics are nonlinear and are given by:

\[ f_{pp}(x) = \begin{cases} 
\exp \left[ 2 \ln(0.15)(1 - x) \right] & x > 0.5 \\
0.3 & x \leq 0.5 
\end{cases} \]  \hspace{1cm} (B.41)

\section*{B.5 Regenerator}

\subsection*{Energy balance}

The catalyst phase of the fluidized bed is assumed to be perfectly mixed. Heat is generated by the following reactions:

(I) \[ 4H + O_2 \rightarrow 2H_2O \]

(II) \[ 2C + O_2 \rightarrow 2CO \]

(III) \[ C + O_2 \rightarrow CO_2 \]

(IV) \[ 2CO + O_2 \rightarrow 2CO_2 \]

Coke deposited on the catalyst consists of carbon and hydrogen. It is assumed that all of the hydrogen is burnt off in the regenerator. The carbon remaining on the catalyst after regeneration \( (C_{\text{rgc}}) \) is returned to the reactor with the regenerated catalyst, where additional coke is deposited. The quantity of hydrogen present due to new deposition of coke in the reactor and the amount of hydrogen burnt off in the regenerator assuming total conversion, is given by Eqn. (B.51). The heat generated by hydrogen combustion is given by Eqn. (B.46). The quantity of heat produced by reactions I-III is given by Eqn. (B.47).

\[ [(W_{\text{reg}} + W_{pp})c_{pc} + M_I] \frac{dT_{\text{reg}}}{dt} = Q_{in} - Q_{out} \]  \hspace{1cm} (B.42)

\[ Q_{in} = Q_{\text{air}} + Q_H + Q_C + Q_{sc} \]  \hspace{1cm} (B.43)

\[ Q_{out} = Q_{fg} + Q_{rgc} + Q_e \]  \hspace{1cm} (B.44)

\[ Q_{\text{air}} = F_{\text{air}}c_{\text{air}}(T_{\text{air}} - T_{\text{base}}) \]  \hspace{1cm} (B.45)

\[ Q_H = F_H \Delta H_H \]  \hspace{1cm} (B.46)

\[ Q_C = F_{\text{air}}(X_{CO_2,sg}\Delta H_1 + X_{CO_2,sg}\Delta H_2) \]  \hspace{1cm} (B.47)

\[ Q_{sc} = F_{sc}c_{sc}(T_{sc} - T_{\text{base}}) \]  \hspace{1cm} (B.48)
\[ Q_{\text{fs}} = F_{\text{air}} (X_{O_2}c_{PCO} + X_{CO}c_{PCO} + X_{CO_2}c_{PCO} + 0.79c_{PN_2}) \]
\[ + 0.5F_HC_{PN_2}(T_{\text{cyc}} - T_{\text{base}}) \]  
(B.49)

\[ Q_{\text{rge}} = F_{\text{rge}}c_{p_c}(T_{\text{reg}} - T_{\text{base}}) \]  
(B.50)

\[ F_H = F_{sc}(C_{sc} - C_{rge})C_H \]  
(B.51)

Eqn. (B.52) gives the temperature profile above the bed. Catalyst is present above the bed due to carry over, and therefore temperature increases above the bed due to heat generated by reactions I-III. The heat balance between the top of the bed and the inlet of the cyclones is affected by the presence of catalyst in this zone. Empirical equations describing catalyst entrainment are given below:

\[
\frac{dT_{\text{reg}}(z)}{dz} = 0 \quad 0 \leq z \leq z_{\text{bed}}
\]
\[
= \left[ \Delta H_1 \frac{dX_{CO}(z)}{dz} + \Delta H_2 \frac{dX_{CO_2}(z)}{dz} \right] \frac{1}{c_p(z)} \quad z_{\text{bed}} \leq z \leq z_{\text{tot}} \]  
(B.52)

\[
c_p(z) = 0.79c_{PN_2} + X_{CO}(z)c_{PCO} + X_{CO_2}(z)c_{PCO_2} + X_{O_2}(z)c_{PO_3}
\]
\[ + [0.5c_{PN_2}F_H + \delta_zc_{PC}M_e] \frac{1}{F_{\text{air}}} \]  
(B.53)

\[
\delta_z = \begin{cases} 0 & z \geq z_{\text{cyc}} \\ 1 & z < z_{\text{cyc}} \end{cases} \]  
(B.54)

Carbon balance

\[ \frac{dC_{\text{rge}}}{dt} = \left[ \frac{dW_c}{dt} - C_{\text{rge}} \frac{dW_{\text{reg}}}{dt} \right] \frac{1}{W_{\text{reg}}} \]  
(B.55)

\[ \frac{dW_{\text{reg}}}{dt} = F_{sc} - F_{sp} \]  
(B.56)

\[ \frac{dW_c}{dt} = (F_{sc}C_{sc} - F_H) - (F_{sp}C_{rge} + 12F_{\text{air}}(X_{CO}c_{PCO} + X_{CO_2}c_{PCO_2})) \]  
(B.57)

Standpipe inventory balance

Catalyst flows over a weir and into the regenerator standpipe. When the catalyst level in the standpipe is greater than 17 ft (the standpipe height is 20 ft) catalyst flow over the weir is slowed down.

\[ \frac{dW_{sp}}{dt} = F_{sp} - F_{rge} \]  
(B.58)

\[ F_{sp} = f_{sp}\sqrt{A_{sp}(z_{\text{bed}} - z_{sp})} - 4925 - 20(3 - d) \]  
(B.59)

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Mass balance

Mass balances on oxygen, carbon monoxide and carbon dioxide are done in the equations below. The concentrations of carbon monoxide and carbon dioxide in the air entering the regenerator are assumed to be zero. The amount of oxygen available for reactions I-III is that available in the air flow entering the regenerator minus the oxygen consumed in the combustion of hydrogen. The rates of reactions I and II are affected by the volume fraction of the catalyst \( \rho_b(z) \) in the bed and the disengaging zone above the bed.

\[
d = \min \left( 3, \frac{W_{sp}}{h_{sp} - \frac{W_{sp}}{\rho_c A_{sp}}} \right) \quad \text{(B.60)}
\]

\[
L_{sp} = \frac{W_{sp}}{\rho_c A_{sp}} \quad \text{(B.61)}
\]

\[
dX_{O_2}(z) = \left[ 100(-0.5k_1 - k_2)\rho_b(z)C_{reg} - k_3 X_{CO}(z) \right] \frac{X_{O_2}(z)}{v_s} \quad \text{(B.62)}
\]

\[
dX_{CO}(z) = \left[ 100k_1 \rho_b(z)C_{reg} - 2k_3 X_{CO}(z) \right] \frac{X_{O_2}(z)}{v_s} \quad \text{(B.63)}
\]

\[
dX_{CO_2}(z) = -\frac{dX_{O_2}(z)}{dz} - 0.5 \frac{dX_{CO}(z)}{dz} \quad \text{(B.64)}
\]

\[
X_{CO_2}(z) = X_{O_2}(z = 0) - X_{O_2}(z) - 0.5 X_{CO}(z) \quad \text{(B.65)}
\]

\[
X_{O_2}(z = 0) = \frac{1}{F_{air}} \left[ 0.21 F_{air} - 0.25 F_{II} \right] \quad \text{(B.66)}
\]

\[
k_1 = 6.9547 \exp \left( \frac{34000}{(T_{reg}(z) + 459.6)} \right) \quad \text{(B.67)}
\]

\[
k_2 = 0.6915 \exp \left( \frac{25000}{(T_{reg}(z) + 459.6)} \right) \quad \text{(B.68)}
\]

\[
k_3 = 0.6412P_6 \exp \left( \frac{45000}{(T_{reg}(z) + 459.6)} \right) \quad \text{(B.69)}
\]

The output concentrations are converted to appropriate units as given below:

\[
C_{O_2,sg} = \frac{100 F_{air} X_{O_2}}{F_{sg}} \quad \text{(B.70)}
\]

\[
C_{CO,sg} = \frac{(1 \times 10^6)28X_{CO}}{28X_{CO} + 44X_{CO_1} + 32X_{O_2} + 22.12} \quad \text{(B.71)}
\]

Volume fraction of catalyst

In the disengaging section of the regenerator bed, catalyst volume fraction drops off vertically. It is assumed that any entrained catalyst entering the cyclones is removed and
returned to the bed so that $\rho_b(z)$ is zero in the cyclones. Volume fraction of catalyst is given by:

$$\frac{d\rho_b(z)}{dz} = 0; \quad \rho_b(z) = 1 - \epsilon_e; \quad 0 \leq z \leq z_{bed}$$

$$= -1000 F_{air} \rho_b(z)$$

$$= \frac{A_{reg} v_s \rho_c,\text{dilute}}{z_{bed} < z \leq z_{cyc}}$$

$$= 0; \quad \rho_b(z) = 0, \quad z_{cyc} < z$$

$$\epsilon_e = \min \left[ 1, \max \left( \epsilon_f, \epsilon_f + \frac{1.904 + 0.363v_s - 0.048v_s^2}{z_{bed}} \right) \right]$$

Void fraction in the regenerator bed ($\epsilon_f$) is a function of superficial velocity and is given by:

$$\epsilon_f = 0.332 + 0.06v_s$$

**Catalyst entrainment**

The mass flow rate of entrained catalyst leaving the bed is described empirically by:

$$M_e = A_{reg} v_s \rho_c,\text{dilute}$$

$$\rho_c,\text{dilute} = -0.878 + 0.582v_s$$

Superficial velocity is given by:

$$v_s = \frac{F_{reg} + F_{air}}{2} \left( \frac{1}{\rho_g A_{reg}} \right)$$

where,

$$\rho_g = \frac{0.0933 P_6}{T_{reg} + 459.6}$$

**Pressure balance**

The pressure balance in the regenerator assumes ideal gas behavior. The pressure at the bottom of the regenerator ($P_{rb}$), is required in the calculation of the air flow into the regenerator from the air blowers:

$$\frac{dP_6}{dt} = \frac{1}{V_{reg,a}} \left[ R \left( n \frac{dT_{reg}}{dt} + (T_{reg} + 459.6) \frac{dn}{dt} \right) \right]$$

$$\frac{dn}{dt} = F_{air} - F_{eg}$$

$$V_{reg,a} = A_{reg} z_{cyc} - A_{reg} z_{bed}(1 - \epsilon_e)$$
$P_{rgh} = P_6 + \frac{W_{reg}}{144A_{reg}}$  \hfill (B.82)

$\Delta P_{RR} = P_6 - P_4$  \hfill (B.83)

Stack gas flows from the regenerator through the stack gas valve $V_{14}$ as given by:

$$F_{sg} = k_{14} V_{14} \sqrt{P_6 - P_{atm}}$$  \hfill (B.84)

**Bed height**

The regenerator bed height is given empirically by:

$$z_{bed} = \min \left[ z_{cyc}, \left( 2.85 + 0.8v_s + \frac{W_{reg} - \rho_{c,dilute}A_{reg}z_{cyc}}{A_{reg}\rho_{c,dense}} \right) \left( 1 - \frac{\rho_{c,dilute}}{\rho_{c,dense}} \right) \right]$$  \hfill (B.85)

where,

$$\rho_{c,dense} = \rho_{part}(1 - \epsilon_f)$$  \hfill (B.86)

**Air lift calculations**

An increase in the lift air flow rate lowers the density of the catalyst in the lift air pipe which in turn lowers the head, resulting in an increase in catalyst flow through the U-bend. Changes density in the lift pipe occur with an assumed time constant $\tau_{fill}$, and are given by:

$$\frac{d\rho_{lift}}{dt} = \left[ \frac{F_c}{\nu_{cat,lift}\Delta p_{lp}} + \rho_{air} - \rho_{lift} \right] \frac{1}{\tau_{fill}}$$  \hfill (B.87)

where,

$$\rho_{air} = \frac{29P_6}{R(T_{sc} + 459.6)}$$  \hfill (B.88)

$$\nu_{air,lift} = \frac{F_c}{\Delta p_{lp}\rho_{air}}$$  \hfill (B.89)

$$\nu_{cat,lift} = \max \left[ \nu_{air,lift} - \nu_{slip}, \frac{F_c}{\Delta p_{lp}\rho_{part}} \right]$$  \hfill (B.90)

The pressure at the bottom of the lift pipe is the sum of the regenerator pressure, $P_6$, and the heads in the lift pipe and the regenerator bed above the top of the lift pipe:

$$P_{blp} = P_6 + \frac{\rho_{lift}\nu_{lift}}{144} + \frac{(z_{bed} - z_{lp})\rho_{c,dense}}{144}$$  \hfill (B.91)
B.6 Air blowers

Combustion air blower

It is a centrifugal compressor driven by a constant-speed electric motor. Throughput is controlled by a throttling valve ($V_6$) on the compressor inlet line. A head capacity performance equation is provided that relates suction volume as a function of discharge pressure when the suction is at normal atmospheric pressure. To obtain suction flowrates at different suction pressures, it is assumed that the performance curve at any suction pressure is the same as the curve for one atmosphere at the same polytropic head.

The head-capacity performance equation is:

$$F_{\text{sucn,comb}} = 45000 + \sqrt{1.581 \times 10^9 - 1.249 \times 10^6 P_{\text{base}}^2}$$  \hspace{1cm} (B.92)

where,

$$P_{\text{base}} = \frac{14.7 P_2}{P_1}$$  \hspace{1cm} (B.93)

Suction and discharge pressures can be given by:

$$\frac{dP_1}{dt} = \frac{R(T_{\text{atm}} + 459.6)}{29V_{\text{comb,s}}} (F_{V_6} - F_6) = 0$$  \hspace{1cm} (B.94)

$$\frac{dP_2}{dt} = \frac{R(T_{\text{comb,d}} + 459.6)}{29V_{\text{comb,s}}} (F_6 - F_7 - F_{V_1})$$  \hspace{1cm} (B.95)

where,

$$F_6 = \frac{0.04511 F_1 F_{\text{sucn,comb}}}{T_{\text{atm}} + 459.6}$$  \hspace{1cm} (B.96)

$$F_7 = k_{\text{comb}} \sqrt{P_2 - P_{\text{rgb}}}$$  \hspace{1cm} (B.97)

$$F_{V_6} = k_{\theta f_{pp}} (V_6) \sqrt{P_{\text{atm}} - P_1}$$  \hspace{1cm} (B.98)

$$F_{V_1} = k_{\theta f_{pp}} (V_1) \sqrt{P_2 - P_{\text{atm}}}$$  \hspace{1cm} (B.99)

Lift air blower

The lift air blower is a single stage centrifugal compressor driven by a variable speed steam turbine with a speed control governor. A single performance equation is provided that relates polytropic head divided by speed squared and suction volume divided by speed. Suction flow for a given discharge pressure is returned at a specific base speed and then corrected for the actual compressor speed. The performance equation is given by:

$$F_{\text{base}} = 8600 + \sqrt{2.582 \times 10^8 - 1.068 \times 10^5 P_{\text{base,d}}^2}$$  \hspace{1cm} (B.100)
where,
\[
P_{\text{base,d}} = \left[ (P_3^M - P_{\text{atm}}^M) \left( \frac{s_b^2}{s_a^2} \right) + P_{\text{atm}}^M \right]^{1/m} \tag{B.101}
\]
\[
M = \frac{k_{\text{aug}} - 1}{k_{\text{aug}} \eta_p} \tag{B.102}
\]

Lift air flow rate is obtained from:
\[
F_8 = \frac{0.04511 P_f F_{\text{sucn, lift}}}{T_{\text{atm}} + 459.6} \tag{B.103}
\]

where,
\[
F_{\text{sucn, lift}} = F_{\text{base}} \left( \frac{s_a}{s_b} \right) \tag{B.104}
\]
\[
F_{\text{surf, lift}} = 5025 + 112 P_3 \tag{B.105}
\]

Flow rates associated with the lift air blower system and spill air line are:
\[
F_9 = k_{\text{lift}} \sqrt{P_3 - P_{\text{blp}}} \tag{B.106}
\]
\[
F_70 = k_0 V_0 \sqrt{P_3 - P_{\text{atm}}} \tag{B.107}
\]
\[
F_{V_0} = k_0 V_0 \sqrt{P_3 - P_{\text{atm}}} \tag{B.108}
\]
\[
F_{\text{air}} = \frac{F_7 + F_9 + F_{10}}{29} \tag{B.109}
\]
\[
F_t = F_7 + F_9 + F_{10} \tag{B.110}
\]

The discharge pressure and the speed of the lift air blower are given by:
\[
\frac{dP_3}{dt} = \frac{R(T_{\text{lift,d}} + 459.6)}{29 V_{\text{lift}}} (F_8 - F_{V_0} - F_9 - F_{10}) \tag{B.111}
\]
\[
s_a = s_a^{\text{min}} + 1100 V_{\text{lift}} \tag{B.112}
\]

### B.7 Catalyst circulation

Circulation of spent catalyst and regenerated catalyst is modeled as a single phase flow governed by simple force balances. Because the dynamics of the catalyst circulation lines are orders of magnitude faster than other dynamic elements of the FCCU system (notably the regenerator thermal dynamics), a pseudo-steady state assumption is applied to the force balances on the spent and regenerated catalyst lines. Constant friction factors are assumed for each circulation line.
The force balances on the regenerated catalyst U-bend is given by:

\[
\frac{dv_{rgc}}{dt} = \frac{f_{rgc}}{M_{rgc}} = 0
\]  

(B.113)

where,

\[
M_{rgc} = \left[ W_{sp} + (A_{ubend_{rgc}}L_{ubend_{rgc}}\rho_c) \right] / g
\]  

(B.114)

\[
f_{rgc} = \Delta P_{rgc}A_{ubend_{rgc}} - v_{rgc}L_{ubend_{rgc}}f_{ubend_{rgc}}
\]  

(B.115)

\[
\Delta P_{rgc} = 144(P_b - P_{r1}) + \left[ \frac{W_{sp}}{A_{sp}} + (E_{tap} - E_{inlet})\rho_c \right]
\]  

(B.116)

\[
F_{rgc} = v_{rgc}A_{ubend_{rgc}}\rho_c
\]  

(B.117)

The force balance on the spent catalyst circulation line is written as:

\[
\frac{dv_{sc}}{dt} = \frac{f_{sc}}{M_{sc}} = 0
\]  

(B.118)

\[
M_{sc} = \left[ W_{sp} + (A_{ubend_{sc}}L_{ubend_{sc}}\rho_c) \right] / g
\]  

(B.119)

\[
f_{sc} = \Delta P_{sc}A_{ubend_{sc}} - v_{sc}L_{ubend_{sc}}f_{ubend_{sc}}
\]  

(B.120)

\[
\Delta P_{sc} = 144(P_a - P_{blp}) + \left[ \frac{W_r}{A_{stripper}} + (E_{stripper} - E_{liftair})\rho_c \right]
\]  

(B.121)

\[
F_{sc} = v_{sc}A_{ubend_{sc}}\rho_c
\]  

(B.122)

B.8 Symbols

- \( A_{lp} \): Cross sectional area of lift pipe
- \( A_{reg} \): Cross sectional area of regenerator
- \( A_{ris} \): Cross sectional area of reactor riser
- \( A_{sp} \): Cross sectional area of stand pipe
- \( A_{stripper} \): Cross sectional area of reactor stripper
- \( A_{ubend_{rgc}} \): Cross sectional area of regenerated catalyst U-bend
- \( A_{ubend_{sc}} \): Cross sectional area of spent catalyst U-bend
- \( a_1 \): Furnace heat loss parameter (Btu/s °F)
- \( a_2 \): Furnace heat loss parameter (Btu/s)
- \( C_{CO,sg} \): Concentration of carbon monoxide in stack gas (ppm)
- \( C_H \): Weight fraction of hydrogen in coke (lb of \( H_2 \)/lb coke)
- \( C_{O_2,sg} \): Concentration of oxygen in regenerator stack (mol %)
- \( c_p(z) \): Average heat capacity (Btu/mol °F)
- \( c_{air} \): Heat capacity of air (Btu/mol °F)
- \( c_{pc} \): Heat capacity of catalyst (Btu/lb °F)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{\text{PCO}} )</td>
<td>Heat capacity of carbon monoxide (Btu/mol(^\circ)F)</td>
</tr>
<tr>
<td>( c_{\text{CO}_2} )</td>
<td>Heat capacity of carbon dioxide (Btu/mol(^\circ)F)</td>
</tr>
<tr>
<td>( c_{\text{FF}} )</td>
<td>Heat capacity of fresh feed liquid (Btu/lb(^\circ)F)</td>
</tr>
<tr>
<td>( c_{\text{FFV}} )</td>
<td>Heat capacity of fresh feed vapor (Btu/lb(^\circ)F)</td>
</tr>
<tr>
<td>( c_{\text{H}_2\text{O}} )</td>
<td>Heat capacity of steam (Btu/mol(^\circ)F)</td>
</tr>
<tr>
<td>( c_{\text{N}_2} )</td>
<td>Heat capacity of nitrogen (Btu/mol(^\circ)F)</td>
</tr>
<tr>
<td>( c_{\text{O}_2} )</td>
<td>Heat capacity of oxygen (Btu/mol(^\circ)F)</td>
</tr>
<tr>
<td>( c_{\text{SV}} )</td>
<td>Heat capacity of slurry vapor (Btu/lb(^\circ)F)</td>
</tr>
<tr>
<td>( C_{\text{RGC}} )</td>
<td>Weight fraction of coke on spent catalyst (lb coke/lb catalyst)</td>
</tr>
<tr>
<td>( C_{\text{RW}} )</td>
<td>Wet gas compression ratio</td>
</tr>
<tr>
<td>( C_1 )</td>
<td>Wet gas production constant ( (0.0088438 \text{ mol/lb feed}) )</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>Wet gas production constant ( (0.00004 \text{ mol/lb feed deg ( F )}) )</td>
</tr>
<tr>
<td>( E_{\text{lift air}} )</td>
<td>Elevation of regenerator lift air injection (ft)</td>
</tr>
<tr>
<td>( E_{\text{oil inlet}} )</td>
<td>Elevation where oil enters the reactor riser (ft)</td>
</tr>
<tr>
<td>( E_{\text{stripper tap}} )</td>
<td>Elevation of reactor stripper tap (ft)</td>
</tr>
<tr>
<td>( E_{\text{tap}} )</td>
<td>Pressure tap elevation on standpipe (ft)</td>
</tr>
<tr>
<td>( F_{\text{AIR}} )</td>
<td>Air flow rate into regenerator (mol/s)</td>
</tr>
<tr>
<td>( F_{\text{B}} )</td>
<td>Effect of feed type on coke production</td>
</tr>
<tr>
<td>( F_{\text{base}} )</td>
<td>Air lift compressor inlet suction flow at base conditions (ICFM)</td>
</tr>
<tr>
<td>( F_{\text{coke}} )</td>
<td>Production of coke in reactor riser (lb/s)</td>
</tr>
<tr>
<td>( F_{\text{GO}} )</td>
<td>Flow of gas oil to reactor riser (lb/s)</td>
</tr>
<tr>
<td>( F_{\text{H}} )</td>
<td>Burning rate of hydrogen (lb/s)</td>
</tr>
<tr>
<td>( f_{\text{OF}} )</td>
<td>Overflow factor</td>
</tr>
<tr>
<td>( f_{\text{OP}(x)} )</td>
<td>Nonlinear valve flowrate function</td>
</tr>
<tr>
<td>( f_{\text{RGC}} )</td>
<td>Force exerted by regenerated catalyst (lb(_f))</td>
</tr>
<tr>
<td>( F_{\text{RRC}} )</td>
<td>Flow rate of regenerated catalyst (lb/s)</td>
</tr>
<tr>
<td>( f_{\text{SC}} )</td>
<td>Force exerted by spent catalyst (lb(_f))</td>
</tr>
<tr>
<td>( F_{\text{SC}} )</td>
<td>Flow rate of spent catalyst (lb/s)</td>
</tr>
<tr>
<td>( F_{\text{SG}} )</td>
<td>Stack gas flow (mol/s)</td>
</tr>
<tr>
<td>( F_{\text{SP}} )</td>
<td>Flow in standpipe (lb/s)</td>
</tr>
<tr>
<td>( F_{\text{SUN,comb}} )</td>
<td>Combustion air blower inlet suction flow (ICFM)</td>
</tr>
<tr>
<td>( F_{\text{SUN, lift}} )</td>
<td>Lift air blower inlet suction flow (ICFM)</td>
</tr>
<tr>
<td>( F_{\text{SUN, sug}} )</td>
<td>Wet gas compressor inlet suction flow (ICFM)</td>
</tr>
<tr>
<td>( F_{\text{SURGE, comb}} )</td>
<td>Combustion air blower surge flow (ICFM)</td>
</tr>
<tr>
<td>( F_{\text{SURGE, lift}} )</td>
<td>Lift air blower surge flow (ICFM)</td>
</tr>
<tr>
<td>( F_{\text{SURGE, sug}} )</td>
<td>Wet gas compressor surge flow (ICFM)</td>
</tr>
<tr>
<td>( F_{\text{T}} )</td>
<td>Total air flow into the regenerator (lb/s)</td>
</tr>
<tr>
<td>( f_{\text{UBEND, RGC}} )</td>
<td>Regenerated catalyst friction factor (lb s/ft(^2))</td>
</tr>
<tr>
<td>( f_{\text{UBEND, SC}} )</td>
<td>Spent catalyst friction factor (lb s/ft(^2))</td>
</tr>
<tr>
<td>( F_{V_6} )</td>
<td>Flow through combustion air blower suction valve ( (V_6) ) (lb/s)</td>
</tr>
<tr>
<td>( F_{V_7} )</td>
<td>Flow through combustion air blower vent valve ( (V_7) ) (lb/s)</td>
</tr>
<tr>
<td>( F_{V_8} )</td>
<td>Flow through lift air blower vent valve ( (V_8) ) (lb/s)</td>
</tr>
</tbody>
</table>
$F_{V_{11}}$ Flow through wet gas compressor suction valve ($V_{11}$) (lb/s)
$F_{V_{12}}$ Flow through wet gas flare valve ($V_{12}$) (lb/s)
$F_{V_{13}}$ Flow through wet gas compressor anti-surge valve ($V_{13}$) (lb/s)
$F_{W}$ Wet gas production in reactor (mol/s)
$F_{1}$ Flow of wash oil to reactor riser (lb/s)
$F_{set}$ Setpoint to wash oil flow controller (lb/s)
$F_{2}$ Flow of diesel oil to reactor riser (lb/s)
$F_{set}$ Setpoint to diesel oil flow controller (lb/s)
$F_{3}$ Flow of fresh feed to reactor riser (lb/s)
$F_{set}$ Setpoint to fresh feed flow controller (lb/s)
$F_{4}$ Flow of slurry to reactor riser (lb/s)
$F_{set}$ Setpoint to slurry flow controller (lb/s)
$F_{5}$ Flow of fuel to furnace (lb/s)
$F_{set}$ Setpoint to fuel flow controller (lb/s)
$F_{6}$ Combustion air blower throughput (lb/s)
$F_{7}$ Combustion air flow to the regenerator (lb/s)
$F_{8}$ Lift air blower throughput (lb/s)
$F_{9}$ Lift air flow to the regenerator (lb/s)
$F_{10}$ Spill air flow to the regenerator (lb/s)
$F_{11}$ Wet gas flow to the vapor recovery unit (mol/s)
$g$ Acceleration due to gravity ($lbm/s^2 lb_f$)
$h_{lift}$ Height of lift pipe (ft)
$h_{ris}$ Height of reactor riser (ft)
$h_{exp}$ Height of regenerator standpipe (ft)
$H_{wg}$ Wet gas compressor head (psia)
$k_{avg}$ average ratio of specific heats
$k_{comb}$ Combustion air blower discharge pipe flow resistance factor (lb/s√psia)
$k_1$ Reaction rate constant of reaction I (1/s)
$k_2$ Reaction rate constant of reaction II (1/s)
$k_3$ Reaction rate constant of reaction III (mol air/s mol CO)
$k_6$ Combustion air blower suction valve flow rating (lb/s√psia)
$k_7$ Combustion air blower vent valve flow rating (lb/s√psia)
$k_8$ Lift air blower vent valve flow rating (lb/s√psia)
$k_9$ Lift air blower spill valve flow rating (lb/s√psia)
$k_{11}$ Wet gas compressor suction valve flow rating (mol/s√psia)
$k_{12}$ Wet gas flare valve flow rating (mol/s√psia)
$k_{13}$ Wet gas compressor anti-surge valve flow rating (mol/s√psia)
$k_{14}$ Regenerator stack gas valve flow rating (mol/s√psia)
$L_{sp}$ Level of catalyst in standpipe (ft)
$L_{rubend_{reg}}$ Length of regenerated catalyst U-bend (ft)
$L_{rubend_{sp}}$ Length of spent catalyst U-bend (ft)
$M$ Polytropic exponent
\( MC_{p,eff} \) Effective heat capacity of riser vessel and catalyst (Btu/deg F)
\( M_e \) Flow rate of entrained catalyst from dense bed into dilute phase (lb/s)
\( M_i \) Effective heat capacity of regenerator mass (Btu/deg F)
\( M_{gc} \) Inertial mass of regenerated catalyst (lb \( s^2/ft \))
\( M_{sc} \) Inertial mass of spent catalyst (lb \( s^2/ft \))
\( n \) Quantity of gas (mol)
\( P_{atm} \) Atmospheric pressure (psia)
\( P_{base} \) Combustion air blower base discharge pressure (psia)
\( P_{base,d} \) Lift air blower base discharge pressure (psia)
\( P_{blp} \) Pressure at bottom of lift pipe (psia)
\( P_b \) Pressure at bottom of reactor riser (psia)
\( P_{rgb} \) Pressure at bottom of regenerator (psia)
\( P_{rru} \) Discharge pressure of wet gas compressor to vapor recovery unit (psia)
\( P_1 \) Combustion air blower suction pressure (psia)
\( P_2 \) Combustion air blower discharge pressure (psia)
\( P_3 \) Lift air blower discharge pressure (psia)
\( P_a \) Reactor pressure (psia)
\( P_e \) Regenerator pressure (psia)
\( P_7 \) Wet gas compressor suction pressure (psia)
\( Q_{air} \) Enthalpy of air to regenerator (Btu/s)
\( Q_c \) Total heat of burning carbon (Btu/s)
\( Q_{catout} \) Enthalpy of catalyst out of reactor riser (Btu/s)
\( Q_{cracking} \) Heat generated from cracking (Btu/s)
\( Q_e \) Total heat loss from regenerator to environment (Btu/s)
\( Q_{ff} \) Heat required to bring fresh feed to reactor riser temperature (Btu/s)
\( Q_{fr} \) Heat required to raise fresh feed temperature from 700 deg F (liq) to 1000 deg F (vap) (Btu/lb)
\( Q_H \) Enthalpy of hydrogen to regenerator (Btu/s)
\( Q_{in} \) Enthalpy into regenerator (Btu/s)
\( Q_{out} \) Enthalpy out of regenerator (Btu/s)
\( Q_{loss} \) Heat loss from furnace (Btu/s)
\( Q_{rgc} \) Enthalpy regenerated catalyst (Btu/s)
\( Q_{sc} \) Enthalpy spent catalyst (Btu/s)
\( Q_{slurry} \) Enthalpy required to bring slurry to reactor riser temperature (Btu/s)
\( Q_{sr} \) Heat required to raise slurry temperature from 500 deg F (liq) to 1000 deg F (vap) (Btu/lb)
\( R \) Universal gas constant (ft³ psia/lb-mol deg R)
\( s_a \) Actual speed of the lift air blower (rpm)
\( s_{a,max} \) Maximum speed of the lift air blower (6300 rpm)
\( s_{a,min} \) Minimum speed of the lift air blower (5000 rpm)
\( s_b \) Base speed of the lift air blower (5950 rpm)
\( t \)  
\( T_{\text{air}} \) Temperature of air entering regenerator (deg F)  
\( T_{\text{atm}} \) Atmospheric temperature (deg F)  
\( T_{\text{base}} \) Base temperature (1100 deg F)  
\( T_{\text{base, f}} \) Base temperature of reactor fresh feed (700 deg F)  
\( T_{\text{comb}, d} \) Combustion air blower discharge temperature (190 deg F)  
\( T_{\text{cyc}} \) Regenerator stack gas temperature at cyclone (deg F)  
\( T_{\text{diff}} \) Temperature difference between cyclone and regenerator bed temperature (deg F)  
\( T_{\text{lift}, d} \) Lift air blower discharge temperature (225 deg F)  
\( T_{\text{lm}} \) Furnace log mean temperature difference (deg F)  
\( T_r \) Temperature of reactor riser (deg F)  
\( T_{\text{ref}} \) Base temperature for reactor riser energy balance (999 deg F)  
\( T_{\text{reg}} \) Temperature of regenerator bed (deg F)  
\( T_{\text{sc}} \) Temperature of spent catalyst entering regenerator (deg F)  
\( T_1 \) Temperature of fresh feed entering furnace (deg F)  
\( T_2 \) Temperature of fresh feed entering reactor riser (deg F)  
\( T_{2, ss} \) Steady state furnace outlet temperature (deg F)  
\( T_3 \) Furnace firebox temperature (deg F)  
\( U_A_f \) Furnace overall heat transfer coefficient (Btu/s)  
\( v_{\text{air, lift}} \) Velocity of air in lift pipe (ft/s)  
\( v_{\text{cat, lift}} \) Velocity of catalyst in lift pipe (ft/s)  
\( V_{\text{comb}, d} \) Combustion air blower discharge system volume (1000 ft\(^3\))  
\( V_{\text{comb}, s} \) Combustion air blower suction system volume (200 ft\(^3\))  
\( V_{\text{lift}} \) Manipulated variable for lift air blower steam valve (0-1.2)  
\( V_{\text{lift}, d} \) Lift air blower discharge system volume (200 ft\(^3\))  
\( V_{\text{reg, g}} \) Regenerator volume occupied by gas (ft\(^3\))  
\( v_{\text{reg}} \) Velocity of regenerated catalyst (ft/s)  
\( v_{\text{ris}} \) Volumetric flowrate in reactor riser (ft\(^3\)/s)  
\( u_s \) Superficial velocity in regenerator (ft/s)  
\( v_{\text{sc}} \) Velocity of spent catalyst (ft/s)  
\( v_{\text{slip}} \) Slip velocity (2.2 ft/s)  
\( V_6 \) Combustion air blower suction valve position  
\( V_7 \) Combustion air blower vent valve position  
\( V_8 \) Lift air blower vent valve position  
\( V_9 \) Spill air valve position  
\( V_{11} \) Wet gas compressor suction valve position  
\( V_{12} \) Wet gas flare valve position  
\( V_{13} \) Wet gas compressor vent valve position  
\( V_{14} \) Stack gas valve position  
\( W_c \) Inventory of carbon in regenerator (lb)  
\( W_r \) Inventory of catalyst in reactor (lb)  
\( W_{\text{reg}} \) Inventory of catalyst in regenerator (lb)
The table contains the following variables:

- $W_{\text{ris}}$: Inventory of catalyst in reactor riser (lb)
- $W_{\text{reg}}$: Inventory of catalyst in regenerator standpipe (lb)
- $WHHSV$: Weight hourly space velocity (lb oil/lb cat/h)
- $X_{\text{CO}}$: Molar ratio of CO to air
- $X_{\text{CO,sg}}$: Molar ratio of CO to air in stack gas
- $X_{\text{CO}_2}$: Molar ratio of $CO_2$ to air
- $X_{\text{CO}_2,sg}$: Molar ratio of $CO_2$ to air in stack gas
- $X_{\text{N}_2}$: Molar ratio of $N_2$ to air
- $X_{\text{O}_2}$: Molar ratio of $O_2$ to air
- $X_{\text{O}_2,sg}$: Molar ratio of $O_2$ to air in stack gas
- $z$: Vertical position in regenerator (ft)
- $z_{\text{bed}}$: Regenerator dense bed height (ft)
- $z_{\text{cyc}}$: Height of cyclone inlet (ft)
- $z_{\text{lp}}$: Height of lift pipe discharge (ft)
- $z_{\text{sp}}$: Standpipe exit height from bottom of regenerator (ft)
- $z_{\text{top}}$: $O_2, CO_2$ measurement point (ft)

Greek symbols:

- $\delta_z$: Dirac delta function
- $\Delta H_{\text{crack}}$: Heat of cracking (Btu/lb)
- $\Delta H_{f u}$: Heat of combustion of furnace fuel (Btu/SCF)
- $\Delta H_H$: Heat of combustion of hydrogen (Btu/lb)
- $\Delta H_1$: Heat of formation of CO (Btu/mol of CO produced)
- $\Delta H_2$: Heat of formation of $CO_2$ (Btu/mol of $CO_2$ produced)
- $\Delta P_{\text{frac}}$: Pressure drop across reactor fractionator (psia)
- $\Delta P_{\text{rgc}}$: Pressure drop from bottom of standpipe to oil inlet elevation of reactor riser (psia)
- $\Delta P_{\text{RR}}$: Differential pressure between regenerator and reactor = $P_6 - P_4$, (psia)
- $\Delta P_{\text{pc}}$: Pressure drop from bottom of reactor to lift air injection elevation (psia)
- $\Delta T_{\text{stripper}}$: Temperature drop across reactor stripper (deg F)
- $\epsilon_e$: Effective void fraction in regenerator dense phase bed
- $\epsilon_f$: Apparent void fraction in regenerator dense phase bed
- $\eta_p$: Polytropic efficiency
- $\rho_{\text{airg}}$: Density of air at regenerator conditions (lb/ft$^3$)
- $\rho_B$: Volume fraction of catalyst
- $\rho_c$: Density of catalyst in U-bend and regenerator (lb/ft$^3$)
- $\rho_{c,\text{dilute}}$: Density of catalyst in the dilute phase (lb/ft$^3$)
- $\rho_{c,\text{dense}}$: Density of catalyst in the dense bed (lb/ft$^3$)
- $\rho_g$: Density of exit gas (mol/ft$^3$)
- $\rho_{\text{lift}}$: Density of catalyst in lift pipe (lb/ft$^3$)
- $\rho_{\text{part}}$: Settled density of catalyst (lb/ft$^3$)
- $\rho_{\text{ris}}$: Average density of material in reactor riser (lb/ft$^3$)
\( \rho_v \)  Vapor density at reactor riser conditions (lb/ft\(^3\))
\( \tau_{fb} \)  Furnace firebox time constant (s)
\( \tau_{fill} \)  Riser fill time (s)
\( \tau_{fo} \)  Furnace time constant (s)
\( \tau_r \)  Catalyst residence time in riser (min)
\( \Psi_f \)  Effective coke factor for gas-oil feed
Appendix C

FCCU Simulation

C.1 Introduction

The simulation for FCCU and CSTRs was written in C++ for Unix environment. A disk with the raw code, executable, and sample data files is attached to the back cover. The FCCU files are in an extractable file called FCCU.tar.gz. To extract the files, upload the file FCCU.tar.gz to a unix environment machine and type the following commands:

```bash
>>> mv FCCU.tar.gz FCCU.tar.gz < ENTER >
>>> gunzip FCCU.tar.gz < ENTER >
>>> tar-xvf FCCU.tar < ENTER >
```

This will extract all the files required for simulation in a subdirectory called FCCU in the current directory.

- `control.c`: Source code containing all the control related classes implementation
- `modelobj.c`: Source code containing the generic model related class implementation
- `fccmodl.c`: Source code containing the FCC model
- `fcc_cost.c`: Source code containing the FCC cost model and SMCO implementation
- `inverse.c`: Source code containing the matrix inverting routine
- `matrix.c`: Source code containing the matrix operations routine
- `control.h`: Header file for control.c; defines classes for control
- `modelobj.h`: Header file for modelobj.c; defines class for generic model
- `fccmodl.h`: Header file for fccmodl.c; defines class for FCC model
- `fcc_cost.h`: Header file for fcc_cost.c; defines class for FCC cost model
- `matrix.h`: Header file for matrix.c; defines class for matrix
- `base.state`: Data file containing the base case for FCCU before SMCO optimization
- `optim.state`: Data file containing the optimal case for FCCU after SMCO optimization
- `main`: Executable file which runs the FCCU optimization simulation.
- `Makefile`: Utility file to recompile the files mentioned above and form a new executable called `main`. 

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The files '*.o' are the object files of the '*.c' files, and are used for linking and creating the executable file *main*. Once the files have been extracted, the file FCCU.tar.gz can be deleted.

C.2 Class Hierarchy

Figure C.1 shows the C++ class hierarchy in the simulation. The member functions are shown in each class and their names are self-explanatory. A derived class (points to its base class or parent class in the figure) and has access to all the data and the member functions of the parent class.

C.3 General Information

The dynamic simulation for the SMCO application of FCCU can be run by typing *main* at the command prompt and directing the output either to a file or to the screen

```
>> main
```

will direct the output to the screen

```
>> main > (filename)
```

will direct the output to the file *(filename)*

Simulation ending time, timestep, tolerance, SMCO sample time etc. can be set in the file *main.c*. The disturbances, the setpoint changes or the switching of SMCO to *on* can be introduced in the simulation through *main.c*. The base case for the FCCU simulation can be loaded by changing the appropriate line in *main.c* to

```
Model->LoadOptimumSMCOSettings("base.state");
```

The *main.c* can be edited in the Unix environment using any standard editor. The executable file can be rebuilt by typing the command *make*. This command looks for the file called *Makefile* in the current directory.
Figure C.1: C++ Class Hierarchy for FCC Simulation
Appendix D

CSTR Simulation

D.1 Introduction

The simulation for CSTRs was written in C++ for Unix environment. A disk with the raw code, executable, and sample data files is attached to the back cover. The CSTR files are in a extractable file called CSTR.tar.gz. To extract the files, upload the file CSTR.tar.gz to a unix environment machine and type the following commands:

```bash
>> mv CSTR.tar.gz CSTR.tar.gz < ENTER >
>> gunzip CSTR.tar.gz < ENTER >
>> tar -xvf CSTR.tar < ENTER >
```

This will extract all the files required for simulation in two subdirectories called CSTR-IRREV and CSTR-REV in the current directory, for irreversible reaction CSTR simulation and reversible reaction CSTR simulation respectively.

Common files to both Irreversible and Reversible reactions

- **controL.c** Source code containing all the control related classes implementation
- **modelobj.c** Source code containing the generic model related class implementation
- **inverse.c** Source code containing the matrix inverting routine
- **matrix.c** Source code containing the matrix operations routine
- **controL.h** Header file for controL.c; defining classes for control
- **modelobj.h** Header file for modelobj.c; defining class for generic model
- **matrix.h** Header file for matrix.c; defining class for matrix
- **main** Executable file which runs the CSTR optimization simulation.
- **Makefile** Utility file to recompile the files mentioned above and form a new executable called main.
Irreversible Reaction CSTR

- **cstrmodl.c**: Source code containing the CSTR irreversible reaction model
- **cstrcost.c**: Source code containing the CSTR irreversible reaction cost model and SMCO+OSGI implementation
- **cstrmodl.h**: Header file for cstrmodl.c; defining class for CSTR irreversible reaction model
- **cstrcost.h**: Header file for cstrcost.c; defining class for CSTR irreversible reaction cost model

Reversible Reaction CSTR

- **cstrmodl.c**: Source code containing the CSTR reversible reaction model
- **cstrcost.c**: Source code containing the CSTR reversible reaction cost model and SMCO+OSGI implementation
- **cstrmodl.h**: Header file for cstrmodl.c; defining class for CSTR reversible reaction model
- **cstrcost.h**: Header file for cstrcost.c; defining class for CSTR reversible reaction cost model

The files '*.o' are the object files of the '*.c' files, and are used for linking and creating the executable file *main*. Once the files have been extracted, the file CSTR.tar.gz can be deleted.

### D.2 Class Hierarchy

Figure D.1 shows the C++ class hierarchy in the simulation. The member functions are shown in each class and their names are self-explanatory. A derived class (points to its base class or parent class in the figure) and has access to all the data and the member functions of the parent class.

### D.3 General Information

The dynamic simulation for the SMCO application of CSTR can be run by typing `main` at the command prompt and directing the output either to a file or to the screen:

- `>> main` will direct the output to the screen
- `>> main > (filename)` will direct the output to the file *(filename)*

Simulation ending time, timestep, tolerance, SMCO sample time etc. can be set in the file `main.c`. The disturbances, the setpoint changes or the switching of SMCO to *on* can be introduced in the simulation through `main.c`. The perturbations required for OSGI can be introduced by setting the variable PERTURB = 1 in `main.c`. One can also change the period and duration of PRBS signal in `main.c`. The `main.c` can be edited in the Unix environment using any standard editor. The executable file can be rebuilt by typing the command `make`. This command looks for the file called *Makefile* in the current directory.
Figure D.1: C++ Class Hierarchy for CSTR Simulation
Vita

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DOCTORAL EXAMINATION AND DISSERTATION REPORT

Candidate: Umesh K. Chitnis

Major Field: Chemical Engineering

Title of Dissertation: On-Line Steady-State Gain Identification for On-Line Optimization of Multivariable Constrained Chemical Processes

Date of Examination: November 1, 1996

EXAMINING COMMITTEE:

Approved:

Major Professor and Chairman

Dean of the Graduate School

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