CHAPTER 2

PROCESS DESCRIPTION

2.1 INTRODUCTION

In this chapter the MIBK process that requires a closed-loop SID methodology is described. In order to place this process in context, a brief overview of the industry in which this process is used is given in Section 2.2. To give an idea of the complexity of the plant and the importance of the process, the process itself is discussed in a simplified manner in Section 2.3. The controller, called DMCplus, that controls this plant is then described in Section 2.4. Lastly, other relevant process information, which is needed to design and implement the closed-loop SID methodology, is discussed in Section 2.5. This information includes a description of the original identified process model and the measured data sets that were used in the identification process.

Furthermore, because the plant in question is controlled by an MPC controller, an overview of MPC controllers is included in Section 2.4. The characteristics of these controllers are taken into account when the identification methodology is chosen.

2.2 OVERVIEW OF THE INDUSTRY

The particular process for which the closed-loop SID methodology was developed is used within Sasol Limited. The Sasol group of companies comprises diversified fuel, chemical and related manufacturing and marketing operations. Sasol has interests in oil and gas exploration and production, in crude oil refining and liquid fuels marketing. Its principal feedstocks are obtained from coal. The company converts this coal into value-added hydrocarbons through Fischer-Tropsch process technologies [23].

During their first three decades, Sasol's primary goal was to produce high-quality synthetic fuels from coal for the local market. During the 1990s, Sasol's interests have been shifting towards developing higher-value chemicals for a wider spectrum of applications [23].

Currently, Sasol comprises of several main operating companies. One of these companies is SCI in Sasolburg. This company manufactures more than 200 chemical products, e.g.

ammonia, fertilisers, explosives, linear alpha olefins, carbon and tar products, plastics and a broad range of solvents [23]. These products are derived principally from the benefaction of coal at Sasolburg and from various feedstocks purchased from Sasol Synthetic Fuels (SSF) in Secunda.

2.3 OPERATIONAL DESCRIPTION OF THE MIBK PROCESS

A very simplified representation of the MIBK process at SCI in Sasolburg is given in Fig. 2.1. This figure shows that this process consists of two reactors and five distillation columns. For simplicity, the reboilers, which provide the necessary vaporization for the distillation processes, the reflux drums, which hold the condensed vapour from the top of the columns so that liquid (reflux) can be recycled back to the columns, the heat exchangers, valves, pumps and sensors, are not shown in Fig. 2.1 [24].

The purpose of the distillation columns is to separate liquid substances of different densities, using the difference in boiling points. Carefully judged heating evaporates only the lighter substances and subsequent cooling of the resulting gas condenses it back to a liquid [24]. The reactors are industrial plants that provide the right physical conditions for specific chemical reactions to take place [23].

Process Feed: The plant was designed to produce MIBK from the feedstock, Dimethyl Ketone (DMK). DMK, also called acetone, is a manufactured chemical that is found in the natural environment as well. However, industrial processes contribute more acetone to the environment than natural processes. It is a colourless liquid with a distinct smell and taste. It evaporates easily, is flammable and dissolves in water [25].

Export quality acetone, produced by SSF, is received daily by road tanker from Secunda and is off-loaded in Sasolburg. The DMK is then transferred via pump to the surge tank, shown in Fig. 2.1. Unreacted DMK, from the DMK column, is also recycled to this tank [26].

Reactor Section: DMK is fed to the reactors and heated to the reaction temperature with feed-effluent exchangers and steam heaters. The feed is split equally between the two reactors. The reactors are of tubular design, with each tube filled with a catalyst and the feed flowing from top to bottom. The shell side of each reactor is divided into three baffled sections through which tempered water flows. This water controls the reaction temperature by heating or cooling the reaction mixture. The temperature and flow rate of the water to each section are controlled.

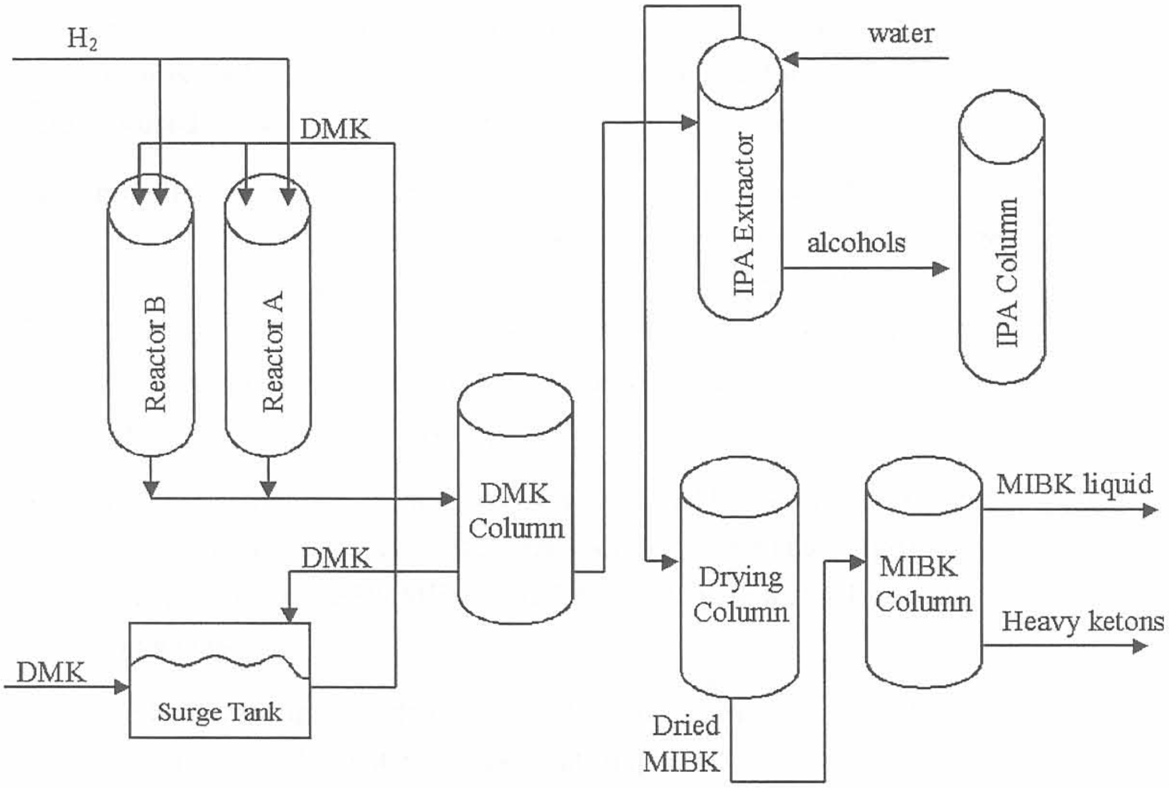

Figure 2.1: A simplified representation of the MIBK process.

Hydrogen is fed via piston compressors to the reactors. The reactor inlets are pressure controlled. The excess hydrogen is flared.

The reaction product collects in the bottom of the reactors. From here it flows under level control to the reactor feed/effluent exchangers, then to the reactor effluent separator and on to the distillation section [26].

Tempered Water System: A closed, circulating tempered water system is used to control the reaction temperatures. Hot water from the reactors is collected in hot water accumulators. The flow from the accumulators is split into two streams. One is heated in a steam heater and sent to the lower and middle sections of the reactors to supply heat for the reaction. The other stream is cooled in a cooling exchanger and then sent to the top and middle sections where it is used to cool down the top zone.

The middle zone water temperature is set via a three-way valve. The flow of the hot water to each zone is set on flow control and these are normally not changed. The flows are set sufficiently high to prevent a major rise in temperature. The inlet temperature sets the heat transfer rate in the reaction sections. There are four temperature indicators in each section. The indicator with the highest temperature is usually selected to be controlled. This temperature increases as the catalyst ages [26].

DMK Column: The DMK column recovers unreacted DMK by withdrawing it as a purified side product from the feed stream. It is then recycled back to the surge tank. The feed to the column is approximately 25% MIBK and 75% DMK with a small percentage of water and other components.

The overhead vapour is condensed and collected in the reflux drum. The reflux is returned to the tower. There is also a steam heater that supplies reboil heat. The condensate from the reboiler is removed.

The bottom product containing the MIBK is fed from the DMK column, under level and flow control, to the Isopropyl Alcohols (IPA) extractor [26].

IPA Extractor: The IPA extractor column extracts alcohols and acids from the MIBK stream by using a counter-current liquid extraction with water as the extractant. Fresh water is supplied under flow control, and is removed as the extract phase from the bottom of the tower and then routed to the IPA column.

The MIBK-rich raffinate phase, which is sent to the drying column, is obtained from the top of the tower under pressure control [26].

IPA Column: The aim of the IPA column is to recover the organics from the water and to recover the MIBK that dissolved in the water [26].

Drying Column: The drying column removes the small amounts of water entrained in the MIBK from the extractor. The bottom product, containing the dried MIBK, is routed to the MIBK column [26].

MIBK Column: The drying column bottom product, which is the feed to the MIBK column, contains essentially pure MIBK with some lighter and heavier components. The MIBK is withdrawn in the MIBK column as a side product under ratio control at approximately 85% of the feed flow. A heavy ketones bottom product is withdrawn from the bottom of the MIBK column. The heavy ketones still contain a small percentage of MIBK [26].

There is a worldwide demand for MIBK and most of the product is, therefore, exported. MIBK, which is a colourless liquid with a pleasant odor, has multiple uses: solvent for paints; varnishes; organic syntheses; extraction process (including extraction of uranium); organic syntheses solvent for protective coating; dewaxing of minerals and oils; synthetic flavoring adjacent; etc. [27].

2.4 CONTROLLER

The MIBK plant is controlled by an MPC controller. A general discussion of these controllers is given. DMC controllers are then described and the implementation of the controller on the MIBK plant is discussed.

2.4.1 Model Predictive Controllers in General

MPC is a class of computer control algorithms that explicitly use a process model to predict future plant outputs and compute appropriate control action (new plant input) through on-line (real-time) optimisation of a cost objective over a future horizon, subject to various constraints. Process measurements provide the feedback and, optionally, feedforward element in the MPC structure [1].

Fig. 2.2 shows the structure of a typical MPC system. It shows that a number of options exist for:

- input-output model,

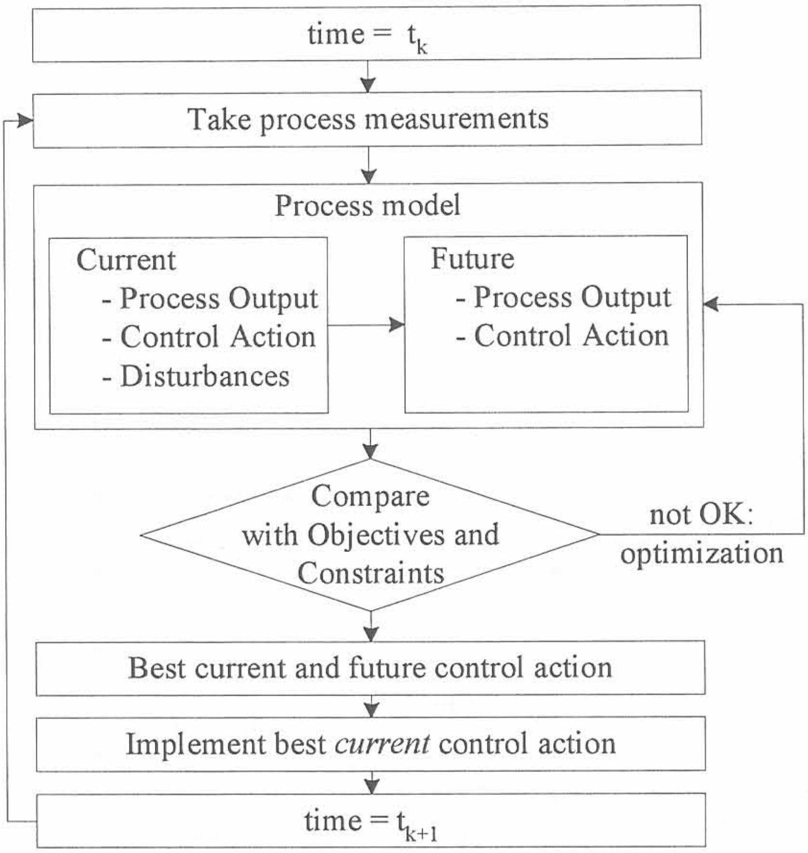

Figure 2.2: The structure of a typical MPC system.

- disturbance prediction,
- prediction and control horizon,
- objective,
- measurement,
- constraints, and
- sampling period (how frequently the on-line optimisation problem is solved) [28].

The possibilities for on-line optimisation are numerous. Fig. 2.2 also shows that the behaviour of an MPC system can be quite complicated, because the control action is determined as the result of the on-line optimisation problem [28].

The MPC control law for the SISO case can most easily be explained by referring to Fig. 2.3. The MIMO case is similar.

For any assumed set of present and future control moves $\Delta u(k)$,$\Delta u(k+1)$,...,$\Delta u(k+i-1)$ the future behaviour of the process outputs $\hat{y}(k+1 \mid k)$, $\hat{y}(k+2 \mid k)$, ..., $\hat{y}(k+h \mid k)$ can

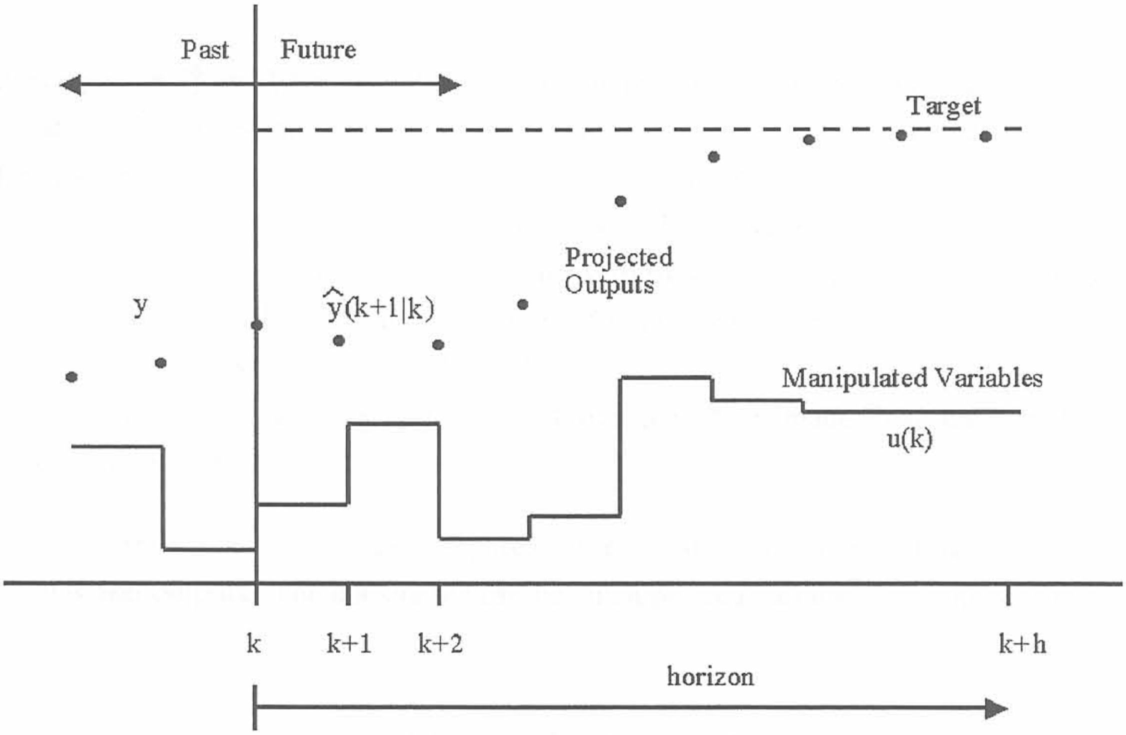

Figure 2.3: The MPC control law [29].

be predicted over a horizon h. The i present and future control moves ($i \leq h$) are computed to minimise a quadratic objective of the form of Eqn. (2.1):

$$\begin{aligned}\min_{\Delta u(k)\ldots\Delta u(k+i-1)} & \sum_{l=1}^{h} \left\|\Gamma_l^y \left[\hat{y}(k+l \mid k) - r(k+l)\right]\right\|^2 \\ & + \sum_{l=1}^{i} \left\|\Gamma_l^u \left[\Delta u(k+l-1)\right]\right\|^2 \text{, where} \\ \|x\|^2 &= \left(\sum_{i=1}^{n} |x_i|^2\right)^{1/2} .\end{aligned} \tag{2.1}$$

In this equation Γ_l^y and Γ_l^u are weighted matrices to penalise particular components of $y(k)$ or $u(k)$ at certain future time intervals. $r(k+l)$ is the, possibly time-varying, vector of future reference values (set-points). Though i control moves are calculated, only the first one, $\Delta u(k)$, is implemented. At the next sampling interval, new values of the measured outputs are obtained, the control horizon is shifted forward by one step and the same computation is repeated. The resulting control law is referred to as *moving horizon* or *receding horizon*. The predicted process outputs $\hat{y}(k+1 \mid k)$, $\hat{y}(k+2 \mid k)$, ..., $\hat{y}(k+h \mid k)$ depend on the measurement $y(k)$, the process model and the assumptions made about the disturbances affecting the outputs [29].

The control action can also be computed subject to hard constraints on the manipulated variables and outputs. The constraints can be: manipulated variable constraints as in Eqn. (2.2)

$$u_{\min}(l) \;\leq\; u(k+l) \leq u_{\max}(l); \tag{2.2}$$

or manipulated variable slew rate constraints as in Eqn. (2.3)

$$|\Delta u(k+l)| \;\leq\; \Delta u_{\max}(l); \tag{2.3}$$

or output variable constraints as in Eqn. (2.4)

$$y_{\min}(l) \;\leq\; \hat{y}(k+l \mid k) \leq y_{\max}(l). \tag{2.4}$$

When hard constraints of this form are imposed, a quadratic programme has to be solved at each time step to determine the control action and the resulting control law is then, generally, nonlinear [29].

2.4.2 Dynamic Matrix Controllers

As mentioned, the DMC controller, which also controls the MIBK plant, is a special type of MPC controller. Key features of the DMC control algorithm include:

- linear step response model for the plant,
- quadratic performance objective over a finite prediction horizon,
- future plant output behaviour specified to follow the set-point as closely as possible, and
- optimal inputs computed as the solution to a Least-Squares Estimate (LSE) problem [1].

The linear step response used by the DMC algorithm relates changes in a process output to a weighted sum of past input changes, referred to as input moves. For the SISO case the step response is represented in Eqn. (2.5):

$$\hat{y}_{k+1} = y_0 + \sum_{j=1}^{h} s_j \Delta u_{k+1-j}. \tag{2.5}$$

The move weights s_j are the step response coefficients and h is the model horizon. Mathematically the step response can be defined as the integral of the impulse response. By using the step response model one can write predicted future output changes as a linear combination of future input moves. The matrix that ties the two together is called a *dynamic matrix* [30].

2.4.3 The DMCplus Controller implemented on the MIBK plant

The marketing strategy for MIBK indicated that every ton of product made can be sold. As a result Sasol's planning objective is to maximise MIBK production at all times.

AspenTech [8] was asked to develop a controller for the MIBK plant with the following objectives in mind:

- maximise production of on-specification MIBK,
- maximise overall yield of MIBK/ton of DMK,
- minimise production of by-products,

- minimise excess hydrogen consumption, and
- minimise energy consumption.

A constrained multivariable DMC controller, called DMCplus, was designed and implemented in September 1998. This controller controls both the reaction and distillation section. Due to slow time constants, a second DMCplus controller was implemented for the slow hexene quality control in the DMK column distillate flow. The second controller has only the distillate flow rate as a manipulated variable. The controllers were joined together with feed-forward variables [26].

2.5 AVAILABLE PROCESS INFORMATION

In this section the original identified process model is described, the measured data sets used in the identification process, is described, and other relevant information regarding the plant and controller is discussed.

2.5.1 Process Model

The process can be modelled as a MIMO system with 56 CVs, and 38 MVs. This model can be represented as a 38x56 matrix with each element representing a SISO model. Luckily this model is partly diagonal (sparse). This means that many of the off-diagonal elements are zero. This property makes it possible to brake down the model into smaller MIMO models that can then be identified separately from the rest of the MVs and CVs.

For this reason only one of these isolated models is used for validation of the developed closed-loop SID methodology in Chapter 4, i.e. an isolated part of reactor A. This part can be modelled as a 4x4 MIMO system [26].

The DMC controller controls the reactor section as follows [26]:

- it tries to keep the temperatures in each zone at their maximum, actuator authority permitting,
- it tries to keep the valves of the condensate flows from saturation,
- it tries to control excess hydrogen flow, and
- it slowly reduces the feed to the reactor if the DMK feed drum level drops too low.

The descriptions and tags of the related CVs considered in the validation process of the proposed closed-loop SID methodology are [26]:

- reactor A zone 1 water inlet temperature valve position (05TIC280A.MV),
- reactor A zone 2 water inlet temperature valve position (05TIC232A.MV),
- reactor A zone 3 water inlet temperature valve position (05TIC279A.MV), and
- reactor A zone 1 water flow valve position (05FIC223A.MV),

The related MVs considered in the validation process are [26]:

- reactor A zone 1 water inlet temperature (05TIC280A.SV),
- reactor A zone 2 water inlet temperature (05TIC232A.SV),
- reactor A zone 3 water inlet temperature (05TIC279A.SV), and
- reactor A zone 1 water flow (05FIC223A.SV),

When AspenTech developed the DMC controller in 1998, open-loop step tests were first conducted in order to identify the MIBK plant [26]. The identified models were stored in step response format. The intention, in this work, is to use these step response models for the comparison and validation of the models identified from the measured process data with the proposed closed-loop SID methodology.

2.5.2 Measured Data

No structured open-loop step tests or any structured closed-loop tests were allowed on the plant. Plant inputs and outputs are however usually logged every 30 seconds. The resulting data sets, logged since 1998, are stored in a database and it was possible to retrieve the desired data.

The logged CVs and MVs of reactor A for October and November 1998 were obtained. This time period was chosen as the controller was commissioned in September 1998, and presumably the plant did not change much from September to November 1998. If this is the case it can be expected that the open-loop identified model from which the controller was designed would be an accurate representation of the plant in October and November. Consequently, the models that were identified by AspenTech before the commissioning of the controller are used to validate the models identified from the closed-loop data, logged during these two months.

Unfortunately, the reference (set-point) values were not logged and, therefore, could not be retrieved. This fact limits the options available for the closed-loop SID methodology.

2.5.3 Other Relevant Information

Concerning the plant and controller, there are a few other relevant remarks to be considered for identification purposes:

The main controller is tuned for a 180 minute time to steady state with an execution time of once every minute to ensure good control for the fast models [26]. The plant data are sampled twice as fast, which means that the plant input-output data sets are inter-sampled by a factor of two.

Unfortunately, not enough information of the controller is available, which implies that the controller cannot be modelled and, therefore, the controller information cannot be used in the identification or validation process.

No disturbance information is available.

There are legally enforced maintenance shutdowns every 36 months, as well as shutdowns every six months to change the catalyst in the reactors. After a shutdown the plant model is usually not accurate any more and a new identified model is desired to ensure optimal long-term controller performance [26].

2.6 CONCLUSION

The MIBK process which was in need of the closed-loop SID methodology is used within a petro-chemical company, Sasol, and was designed to produce MIBK from the feedstock DMK. The process is implemented with reactors, distillation columns, heat exchangers, valves, pumps, sensors, etcetera. The plant is controlled by a DMC controller, which is a type of MPC controller. The DMC algorithm uses a linear step response model to relate changes in a process output to a weighted sum of past input changes, referred to as input moves.

It is clear from the discussion of MPC controllers that the behaviour of the MPC system can be quite complicated, because control actions are determined from the result of an on-line optimisation problem. Hard constraints are also frequently imposed, which results in a quadratic programme that is solved iteratively to determine the control action. The resulting control law is then generally nonlinear. Chapter 4 discusses why these facts restrict the choices in the closed-loop SID methodology.

An isolated part of a reactor that is part of the multivariable MIBK plant was chosen to be used for the validation of the developed closed-loop SID methodology. No structured tests were performed on the plant and logged data sets from normal operation were obtained for the identification process. These sets only contain the input and output signals of the plant. The reference signals are unknown. It is also not possible to model the controller for which no detailed information is available. These facts limit the available options for the closed-loop SID methodology. Since the input-output data sets are inter-sampled, the output inter-sampling approach can be added to the list of options to be considered in the development of the SID methodology.