CHAPTER 1

PROBLEM EXPOSITION

INTRODUCTION

The term “exposition” means an explanatory statement or account, and that is exactly what this chapter aims to achieve. It provides some detail about the origins of, and the rationale behind, the research that is presented in this document.

The first section indicates that the origins of the research that is presented in this document can be traced back to the development of a simulation model of the Sasol East plant. The original simulation model of the Sasol East plant was developed, refined, expanded and maintained over a 3-year time period from 1994 to 1996. The final 1996 simulation model includes the whole Sasol Synfuels complex and makes provision for the investigation of various scenarios. An investigation into the viability to update the final 1996 simulation model, led to an opportunity to use the original simulation modelling method as a point of departure for the development of a generic simulation modelling methodology.

A system description breakdown is provided in the first part of the second section and it is then used to describe the type of system that is considered in this document. To describe a system the physical and functional aspects of the system must be addressed. The physical aspect consists of the system configuration and the characteristics of the elements. The functional aspect consists of the process flow and the process logic. The second part of the section provides the system description of the Synthetic Fuel plant, an imaginary continuous process plant that represents the Sasol East plant.

The third section details the role of simulation modelling as a decision support tool. Simulations are compared to other decision support tools. A simulation model can provide knowledge about past and present system behaviour as well as insight into probable future system behaviour. Managers strive to achieve the maximum possible rate of production or throughput and consequently also the maximum possible profitability. Simulation modelling is a cost-effective way of managing the risk that is associated with decisions.

The shortcomings of the original simulation modelling method are addressed by the fourth section. Some background information is provided on a *Magister* dissertation that is based on the development of the original simulation model. The reasons why a FORTRAN subroutine was included into the original simulation model and the weaknesses of the original method are presented and discussed. These shortcomings were the catalysts that initiated the development of the generic simulation modelling methodology.

The fifth section indicates that the key objective of this research is to develop a generic simulation modelling methodology that can be used to model any generic variant of a stochastic continuous system effectively. The generic methodology renders simulation models that exhibit the following characteristics: short development and maintenance times, user-friendliness, short simulation runtimes, compact size, robustness, accuracy and a single software application.

The importance of the research that is presented in this document is highlighted in the sixth section. The principal range of possible application of the generic simulation modelling methodology falls within the petrochemical industry, but the generic methodology is not restricted to the petrochemical industry alone. Any system that displays the same characteristics as the system that is detailed by the system description in the second section can readily be accommodated by the generic methodology. The majority of simulation software packages cannot adequately accommodate such systems because they focus primarily on the modelling of discrete-event systems.

The last section clarifies the limitations of the generic simulation modelling methodology. Simulation models of the class or type of system that is considered in this document are classified as dynamic, combined, stochastic simulation models. Continuous state change behaviour or transient behaviour is usually represented with state and differential equations. The generic methodology does not accommodate transient behaviour but this is not necessarily a limitation because it simplifies the generic methodology significantly.

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1.1 BACKGROUND INFORMATION

The origins of the research that is presented in this document can be traced back to the development of a simulation model of the Sasol East plant. The Sasol East plant was formerly known as Sasol 3 and it forms part of the Sasol Synfuels (Pty.) Ltd. company. The company will hereafter be referred to simply as Sasol Synfuels. The massive Sasol Synfuels industrial complex is situated at Secunda, South Africa. The following quotation describes the main business activity of Sasol Synfuels (Sasol Synfuels (Proprietary) Limited, 2003):

> "*The company operates the world's only commercial coal-based synfuels manufacturing facility at Secunda. It uses unique Sasol Fischer-Tropsch technology to manufacture synthesis gas from low-grade coal and to convert this into a large range of petrochemical products, including synthetic liquid fuels, industrial pipeline gas and chemical feedstock. These latter products - including ethylene and propylene, ammonia, phenolics, solvents and olefins - form most of the building blocks for the South African chemical and polymer industries.*"

Sasol Synfuels is part of the Sasol group of companies. The Sasol group is the largest publicly listed group in Africa (West, 2003:12).

The need for a simulation model of the Sasol East plant originally arose because the plant management identified the necessity for a decision support tool on a strategic level (Owen, 1994:15,17). In this instance a strategic level is regarded as the level on which decisions of greater possible impact are handled. For example, the decision to move from a 24-month preventive maintenance cycle to a 36-month preventive maintenance cycle may have a pronounced effect on the production and the maintenance of the plant. It is therefore regarded as a strategic level decision. This can be compared to the decision whether to use corrosion prevention surface treatment A or B. Such a decision is regarded as a detail level decision.

In a plant of this size and complexity it is extremely difficult to predict what the effect of a proposed change is going to be on the operation of the plant. The complex interrelationships of the plant, chronological events such as services and random events such as failures can be handled by a simulation model. The simulation model can be used to identify problem areas ("bottlenecks") in the plant and to study the effect of proposed scenarios on the plant. Proposed scenarios may include added capacity at "bottlenecks", changes in the maintenance strategy, *etc.*

The original simulation model of the Sasol East plant was developed, refined, expanded and maintained over a 3-year time period from 1994 to 1996. This relates closely to a comment from Crowe *et al.* (1971:5) to the effect that it may take a few man-years to supply answers to complex problems with a simulation model.

> "*At the other extreme is a very accurate simulation for answering technically sophisticated problems. A simulation to supply such answers may take two to four man-years.*"

The final 1996 simulation model includes both the Sasol East and Sasol West plants as well as some existing and proposed interconnection lines between the two plants. Sasol West was previously known as Sasol 2 and together with Sasol East makes up the bulk of the Sasol Synfuels complex. The interconnection lines are used to channel the production from one plant to the other if required. The final 1996 simulation model makes provision for the evaluation of existing and proposed interconnection lines. It also affords the modeller the opportunity to study the effect of two opposing proposed maintenance strategies on the operation of the Sasol Synfuels complex.

A "phase" service strategy can be compared to a "block" service strategy with the final 1996 simulation model. A "phase" constitutes one half of either of the Sasol East or Sasol West plants, if split lengthwise from the beginning to the end of the process. All in all, there are thus four "phases" in the Sasol Synfuels complex, two "phases" in each of the Sasol East and Sasol West plants. A "block" constitutes any logical subdivision of a "phase". A "phase" service will therefore cause one quarter of the Sasol Synfuels complex to be decommissioned for the duration of the service, while a "block" service will cause one eighth, one sixteenth, *etc.* of the complex to be decommissioned.

From 1996 to 1999 the final 1996 simulation model was in continuous use as a decision support tool. It was used for the evaluation of several different proposed scenarios. During 1999 a concern developed that the final 1996 simulation model (constructed according to a system description or model definition that reflected the 1996 status of the Sasol Synfuels complex) may not accurately reflect the 1999 status of the complex. It was decided to explore the feasibility of updating the final 1996 simulation model to the 1999 status of the Sasol Synfuels complex.

A preliminary feasibility study found that comprehensive changes were needed. Parts of both the Sasol East and Sasol West plants have been dismantled and new additional parts have also been added to both plants. One part of the Sasol West plant was actually destroyed by an explosion and it was prudently decided to redesign the appropriate process. Some of the original feedback-loops have also been moved and new ones added to accommodate new chemical processes that were introduced to increase efficiency and to align product supply with client demand.

The changes that are outlined in the previous paragraph cannot readily be incorporated into the final 1996 simulation model, because the simulation modelling method that is used is not very accommodating when changes of this magnitude are encountered. The simulation modelling method that is used by both the original simulation model of the Sasol East plant and the final 1996 simulation model will be referred to as the original simulation modelling method in the rest of this document. The comprehensive changes that were needed necessitated the proposal of a lengthy and costly process to update the final 1996 simulation model to a 1999 system description or model definition of the Sasol Synfuels complex and consequently the project was cancelled.

Even though the project was shelved, the whole exercise led to a unique opportunity to do something more than just an update of the final 1996 simulation model. It presented a chance to use the original simulation modelling method as a point of departure for the development of a generic simulation modelling methodology. The term "generic" implies that the generic methodology is applicable to an entire class or type that includes all plants or similar systems that exhibit the same characteristics as the Sasol East plant. The generic methodology also effectively addresses the shortcomings of the original method. The investigation into the viability to update the final 1996 simulation model of the Sasol Synfuels complex gave rise to the development of the generic methodology and thus triggered the research that is presented in this document.

In this document the term "method" is used in conjunction with the original simulation modelling method while the term "methodology" is used in conjunction with the generic simulation modelling methodology. In many instances these two terms are perceived to be interchangeable but in the context of this document the term "method" is perceived to be indicative of a lower order terminology, while the term "methodology" is perceived to be indicative of a higher order terminology. Van Dyk (2001:2-4) postulates that the hierarchy of terminologies that is used in Industrial Engineering proceeds along a continuum. The hierarchy that is suggested is as follows: tool, technique, method, approach and philosophy (arranged from lower to higher order). It is suggested that the transition within this hierarchy occurs continually. Even though van Dyk does not make a distinction between the term "method" and the term "methodology", in this document the term "method" is perceived to imply a less elegant, less accomplished procedure with a more restricted range of application, while the term "methodology" is perceived to imply a more elegant, more accomplished procedure with a broader range of application.

Furthermore, the following conventions, regarding the use of the terms "original simulation modelling method" and "generic simulation modelling methodology", are followed:

a) The first reference in a paragraph to the original simulation modelling method uses the term "original simulation modelling method", while subsequent references only use the term "original method".

b) The first reference in a paragraph to the generic simulation modelling methodology uses the term "generic simulation modelling methodology", while subsequent references only use the term "generic methodology".

The aforementioned distinction is necessary to clearly distinguish when the term "method" is used in conjunction with another method that is addressed and when the original simulation modelling method or generic simulation modelling methodology is addressed.

Summary

This section indicates that the origins of this research can be traced back to the development of a simulation model of the Sasol East plant. This simulation model was developed, refined, expanded and maintained over a 3-year time period from 1994 to 1996. The final 1996 simulation model includes the whole Sasol Synfuels complex. In 1999 a concern developed that the final 1996 simulation model may not accurately reflect the 1999 status of the complex. An investigation into the viability to update the final 1996 simulation model, highlighted the shortcomings of the original simulation modelling method and gave rise to the development of the generic simulation modelling methodology.

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1.2 SYSTEM DESCRIPTION

The following exposition of the Sasol East plant gives an indication of the type of system that is considered in this document. A concise definition of a system is provided by Pegden *et al.* (1995:3).

> "*By a* ***system*** *we mean a group or collection of interrelated elements that cooperate to accomplish some stated objective.*"

The "*... a group or collection of interrelated elements ...*" part of the definition refers to the physical aspect of a system while the "*... cooperate to accomplish some stated objective ...*" part of the definition refers to the functional aspect of a system. Both the physical and functional aspects of a system have to be addressed when the system is described.

The physical aspect of a system is described by the configuration of the system and the characteristics of the elements. *The Oxford Compact English Dictionary* (1996:204) describes the term "configuration" as "*an arrangement of parts or elements in a particular form or figure.*" The configuration of the system thus identifies the elements and describes the way that they are arranged and connected. If the system under consideration is a plant, the elements are characterised by their capacities, service schedules and failure characteristics.

The functional aspect of a system is described by the process flow and the process logic of the system. The process flow describes the manner in which "commodities" like data, electrical currents, entities, solids, liquids, gases, *etc.* move or flow through the system. The process part of the process flow describes the processes that the "commodities" are subjected to while the flow part describes the path and the sequence or direction that the "commodities" follow. The process logic describes the rules of operation of the system. For example, if the process flow indicates that coal is supplied by Element(I) to both Element(II) and Element(III), then the rule of operation could stipulate that Element(III) will only be supplied with coal once the capacity of Element(II) is surpassed.

A schematic representation of the system description breakdown that is outlined above is shown in Figure 1.1: *System Description Breakdown*. This approach corresponds with the view of Harrell and Tumay (1999:1) who state that a system consists of resources, activities and controls. The "resources" are the physical aspect of the system, the "activities" are the process flow and the "controls" are the process logic (see the graphical representation of this view in Figure 1.1).

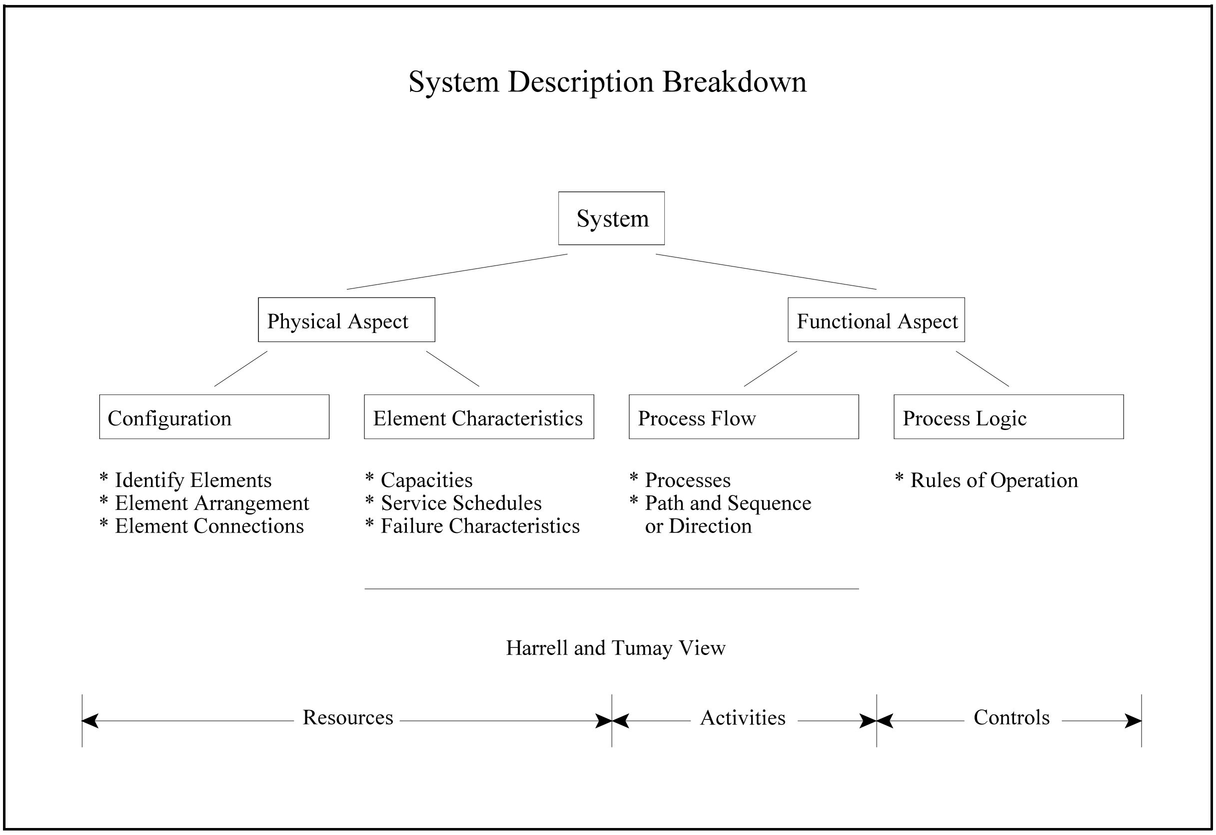


Figure 1.1: System Description Breakdown

The Sasol East plant is a continuous process plant (*i.e.* a system) that produces chemical products from coal. The physical and functional aspects of the plant are detailed in the rest of this section. A simplified schematic representation of the plant is shown in Figure 1.2: *Synthetic Fuel Plant*.

For the purpose of this document some changes to the original data pertaining to the Sasol East plant are incorporated to create the imaginary continuous process plant that is represented in Figure 1.2. The imaginary continuous process plant is used to demonstrate the generic simulation modelling methodology and will hereafter be referred to as the Synthetic Fuel plant.

The reasons for the changes to the original data are the following:

a) It protects the client confidentiality of Sasol Synfuels because the company would prefer not to disclose sensitive operational information, such as the capacity of the plant, to their competition.

b) It makes the representation more generic and representative of any continuous process plant. (Section 1.6 details the possible range of application of the generic simulation modelling methodology in the petrochemical and other industries.)

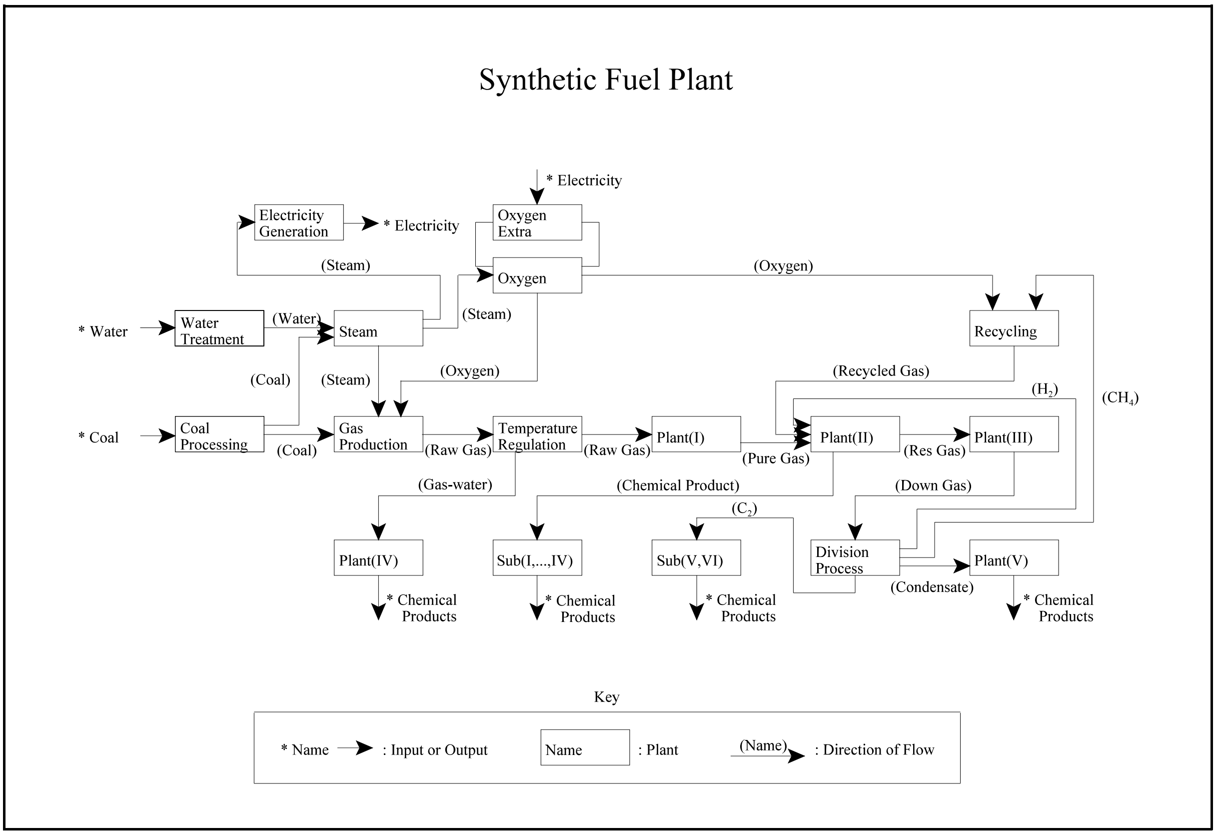


Figure 1.2: Synthetic Fuel Plant

The most obvious change is the change of the name of the plant from the Sasol East Plant to the Synthetic Fuel plant to clearly indicate the move from the specific to the generic. The other changes that are incorporated are the changing of some of the names (of the smaller plants) and the adjustment of all the capacities. For example, the Oxygen plant retains its name *verbatim* because the name is made up of common language words. Proprietary process specific names, on the other hand, are changed to more generic variants like Plant(I), Sub(I), *etc.* The capacities are adjusted by a constant scale factor, implying that the Synthetic Fuel plant is actually a "scale model" of the real Sasol East plant. This gives the added advantage that during the verification and validation of simulation models of the Synthetic Fuel plant the actual results from the Sasol East plant can be adjusted with the same scale factor to create a set of data for verification and validation purposes.

It is important to realise that the term "plant" as used in this document can denote either the Synthetic Fuel plant or one of the smaller plants that make up the Synthetic Fuel plant, depending on the context where it is used. For example, the total Synthetic Fuel plant comprises a number of smaller plants like the Coal Processing plant, the Water Treatment plant, the Steam plant, *etc.*

The configuration of the Synthetic Fuel plant that is represented in Figure 1.2 is exactly the same as that of the Sasol East plant, except for some of the names. The arrangement of the smaller plants and the connections between them are exactly the same as that of the Sasol East plant. The service schedules and failure characteristics, the process flow and the process logic are also not changed. If anything in the system description of the Synthetic Fuel plant is changed, except for the names and the capacities, then the Synthetic Fuel plant will no longer be a "scale model" of the real Sasol East plant.

To summarise, some names and all the capacities are changed, while the arrangement and connections of the smaller plants, the service schedules and failure characteristics, the process flow and the process logic are not changed.

The term "resolution of a model" refers to the level of detail addressed by the model. The level of detail that is required should be chosen in accordance with the objectives of the model. Enough detail should be included to validate any inferences drawn from the use of the model, without making the model cumbersome by the inclusion of unnecessary trivia. Pegden *et al.* (1995:15-16) stress the importance of this approach.

> "*Therefore, the model must include only those aspects of the system relevant to the study objectives.*
>
> *One should always design the model to answer the relevant questions and not to imitate the real system precisely. According to Pareto's law, in every group or collection of entities there exist a vital few and a trivial many. In fact, 80 percent of system behaviour can be explained by the action of 20 percent of its components.*"

The problem is to ensure that the few vital components are identified and included. Crowe *et al.* (1971:177) also warn against the inclusion of unnecessary detail.

> "*The long, detailed computer program has a place in a plant simulation only if meaningless results are generated without it.*"

For the purpose of this document, the Synthetic Fuel plant is considered to consist of 20 smaller plants (some of whom are grouped together for the sake of simplicity in Figure 1.2). The 20 smaller plants are made up of a total of 147 modules. A module can be defined as a grouping of components that has a specific function. For example, in the Gas Production plant the coal is gasified by 40 gasifiers, each consisting of many components. For the resolution that is required in this instance, it is assumed that each individual gasifier represents a module. The Gas Production plant thus has 40 modules. The capacities, services and failures of the gasifier (*i.e.* the module) as an entity are described, not those of the separate components that make up the gasifier. This simplification can be justified by the fact that the requirement is for a decision support tool on a strategic level, not a detail level (see the explanation of strategic versus detail level in the previous section).

In terms of the definition of a system that is provided in the first paragraphs of this section, both the modules and the smaller plants can be considered as elements of the system, just on different levels of resolution. For the purpose of this document the 147 modules are considered as the “lower” level elements of the system and the 20 smaller plants are considered as the “higher” level elements of the system.

The names of the smaller plants are indicated in Figure 1.2 and Column 2 of Table A1: *Number of Modules and Capacities* (see Appendix A: *Synthetic Fuel Plant Detail*). The number of modules in each of the smaller plants is indicated in Column 3 of Table A1.

Some of the smaller plants consist of groupings of different types of modules. The Oxygen plant, for example, consists of three groupings of different types of modules. There are six air turbine and compressor sets, six cold boxes and seven oxygen turbine and compressor sets. For the sake of simplicity the three groupings are referred to as Oxygen-A, -B and -C respectively. The same logic applies to Plant(II) and Plant(IV).

A schematic representation of the Oxygen plant is shown in Figure 1.3: *Oxygen Plant*. It should be clear from the figure that the Oxygen plant actually consists of six parallel lines, each one containing an air turbine and compressor set, a cold box and an oxygen turbine and compressor set. Such a serial, parallel line within a smaller plant is sometimes referred to as a “train”. In this instance the seventh oxygen turbine and compressor set in reality represents a reserve capacity and it was introduced because of the high failure rate of the oxygen turbine and compressor sets.

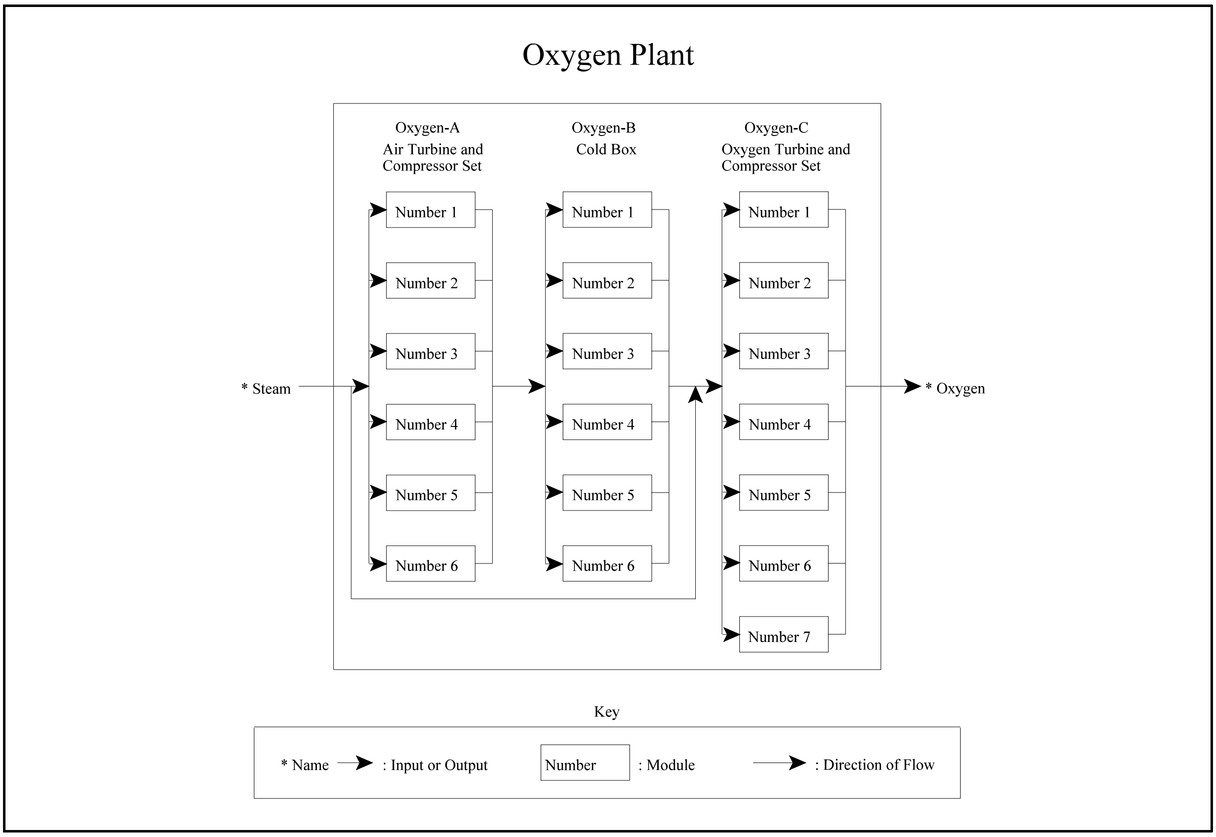


Figure 1.3: Oxygen Plant

The smaller plants have complex switching capabilities. This implies that if one of the modules in a "train" is unavailable (due to service or failure), the whole "train" is not necessarily rendered inoperative. If a module of the same type in another "train" is available, but not in use, it may be incorporated temporarily into the "train" with the unavailable module. Thus an operative "train" may be created from modules that are not positioned in the same geographical parallel line.

The way that the smaller plants are arranged and connected can be derived from Figure 1.2 and Table A1. For example, the Temperature Regulation plant is situated between the Gas Production plant and Plant(I) and connected to the Gas Production plant, Plant(I) and Plant(IV).

That concludes the description of the configuration (element identification, arrangement and connection) of the Synthetic Fuel plant.

The modules are characterised by their capacities, service schedules and failure characteristics. The input and output capacities of the modules are indicated in Columns 4 and 5 respectively of Table A1. The capacities are given as hourly rates of flow for a single module. For example, if the output capacity of each individual module in the Steam plant is 378 ton/h, then the maximum possible output capacity of the Steam plant is 3402 ton/h (nine times 378 ton/h). The coal, water and steam capacities are given in tons per hour (ton/h), the liquid capacities are given in cubic metres per hour (m^3/h) and the gas capacities are given in normalised cubic metres per hour (nm^3/h). Because the temperatures and pressures (and therefore the volumes) of gases differ at different points in the process, the volumes of gases are represented as volumes that are numerically normalised to a standard temperature and pressure. This normalisation makes it possible to compare the volumes of gases at different points in the process.

To summarise, solid phase capacities are given in ton/h (except for water and steam where traditionally the capacities are always given in ton/h), liquid phase capacities are given in m^3/h and gas phase capacities are given in nm^3/h.

The service schedules of the modules are indicated in Table A2: *Service Schedules and Failure Characteristics* (see Appendix A). The services of the modules are strictly chronological events and are characterised by the service cycles of the modules. The service cycles are described by the start times, cycle times and service times (*i.e.* the length of time or duration of the services) of the modules. The cycle times and service times of the modules are indicated in Columns 3 and 4 respectively of Table A2. For example, the modules in the Steam plant are subject to a cycle time of eight weeks (1344 hours) and each service takes 34 hours to complete. The services of the individual modules in the Steam plant are of course staggered in time to minimise the impact of the services on steam production.

Some of the service schedules consist of more than one service cycle. Such an occurrence is referred to as a multiple service cycle. For example, the modules in both the Coal Processing plant and Plant(II)-A have three service cycles that are superimposed on one another. The "phase" services, are services that are conducted on a yearly basis. (A "phase" constitutes one half of the Synthetic Fuel plant, if split lengthwise from the beginning to the end of the process.) There is also a two-yearly shutdown during which routine (mostly statutory) maintenance work is completed.

The failure characteristics of the modules are also indicated in Table A2. The failures of the modules are random (*i.e.* stochastic) events and are characterised by the failure characteristics of the modules. The failure characteristics are described by the failure rates and repair times of the modules.

Various authors indicate that the behaviour of random phenomena can be represented in a model with the help of theoretical probability distributions or empirical (user-defined) distributions (Harrell and Tumay, 1999:83; Kelton *et al.*, 1998:35; Pegden *et al.*, 1995:17; *Simul8*$^{®}$*: Manual and Simulation Guide*, 1999:110). The following quotation from Harrell and Tumay (1999:83) clearly illustrates this:

> "*Random phenomena must be either fit to some theoretical distribution or described using an empirical distribution ...*"

Pegden *et al.* (1995:17-18) provide the following reasons why it is desirable to use a theoretical probability distribution rather than an empirical distribution to represent random behaviour:

a) Using raw empirical data implies that only the past (with its idiosyncrasies) is represented and the only events possible are those that transpired during the period of time when the data were gathered. This is different from the assumption that the basic form of the theoretical probability distribution that represents the data will remain unchanged.

b) It is much easier to change certain aspects of the random behaviour if theoretical probability distributions are used, implying greater flexibility.

c) It is highly desirable to test the sensitivity of the system that is under scrutiny to changes in the random behaviour. This is much easier with theoretical probability distributions than with empirical distributions because of the flexibility of the theoretical probability distributions.

According to Pegden *et al.* (1995:45) the exponential distribution can be used to represent the failure rates of the modules.

> "*The* ***exponential*** *function is widely used for times between independent events such as interarrival times, and lifetimes for devices with a constant hazard rate (when describing the time to failure of a system's component).*"

> "*When the exponential random variable represents time, the distribution possesses the unique property of forgetfulness or lack of memory. Given that* ***T*** *is the time period since the occurrence of the last event, the remaining time,* ***t****, until the next event is independent of* ***T****. Therefore, events for which interarrival times can be represented by the exponential* [distribution] *are said to be completely random.*"

The only value that is needed to describe the exponential distribution is the mean. The mean values of the exponential distributions that represent the failure rates of the modules are indicated in Column 5 of Table A2. These mean values are derived from the failure histories of the modules. The failure histories of the modules are available from the maintenance division of the plant. The mean value of the exponential distribution that represents the failure rate of a module is in fact the Mean Time Between Failure (MTBF) value of the module. The actual failure rate of a module is the reciprocal (*i.e.* the inverse) of the MTBF of the module. For example, the MTBF of the modules in the Steam plant is 2880 hours. It implies that, on average, there will be one failure every four months for each module (*i.e.* every 2880 hours - assume a 30-day month). An exponential distribution with a mean value of 2880 hours can thus be used to represent the failure rate of the modules. The actual failure rate of the modules is the reciprocal of 2880 hours and that is 0,000347 (3,47E-04) failures per hour.

Different theoretical probability distributions can be used to represent the failure rates of components. For example, the best mathematical approximation of the failure rate of a specific component may be a Weibull distribution. Pegden *et al.* (1995:38) indicate that the MTBF of electronic components generally follows a Weibull distribution. Ideally the failure history of each specific component should be subjected to thorough statistical analysis to determine the theoretical probability distribution that provides the best approximation of the failure rate of that specific component. The degree of precision with which the identified theoretical probability distribution approaches the real-world situation, depends largely on the availability and quality of the failure history of that specific component. Harrell and Tumay (1999:83) also stress this point.

> "*To define a distribution using a theoretical distribution requires that the data, if available, be fit to an appropriate distribution that best describes the variable* ..."

The resolution (level of detail) of a model affects the degree of precision required of the theoretical probability distributions that are used to represent the failure rates. The higher the resolution (finer level of detail) of the model, the more effort should be expended to find theoretical probability distributions that represent the failure rates with a high degree of precision.

For the resolution that is required in this instance, the failure rates of the components that make up the modules are not considered. The failure rates of the modules as entities are determined and the exponential distribution is used to represent the failure rates of the modules.

The reasons for this assumption are the following:

a) The requirement is for a decision support tool on a strategic level, not a detail level (see the explanation of strategic versus detail level in the previous section).

b) The quality of the data that make up the failure histories of the modules is suspect in some instances.

According to Pegden *et al.* (1995:45) the triangular distribution can be used to represent the repair times of the modules.

> "*This distribution is most often used when attempting to represent a process for which data are not easily obtained but for which bounds (minimum and maximum) and most likely value (mode) can be established based on knowledge of its characteristics.*"

The triangular distribution is defined by three values, namely: a minimum, a mode and a maximum. The mode is the most likely value or most often occurring value. The three values of the triangular distributions that represent the repair times of the modules are indicated in Columns 6, 7 and 8 of Table A2. These values are derived from the failure histories of the modules. The failure histories of the modules are available from the maintenance division of the plant. Even though the mode of the triangular distribution that represents the repair time of a module is defined as the most likely value of the repair time of the module, it can be likened to the Mean Time To Repair (MTTR) value of the module. In most practical instances, if the triangular distribution is used to represent the repair time of a module, then the MTTR of the module can be used to approximate the mode of the triangular distribution that is used to represent the repair time of the module. The assumption is made that the MTTR and the mode are approximately equal. For example, the minimum repair time of the modules in the Steam plant is 24 hours, the mode or most likely repair time is 120 hours and the maximum repair time is 168 hours.

The same argument applies for the assumption to use the triangular distribution to represent the repair times of the modules, as for the assumption to use the exponential distribution to represent the failure rates of the modules.

The probity of these assumptions is established in Sections 3.6, 3.7 and 4.3 by the verification and validation of the simulation models that use the system description presented in this section as their model definition.

The process flow or activities according to Harrell and Tumay (1999:1) of the Synthetic Fuel plant can be derived from Figure 1.2 and Table A1. For example, the input of the Coal Processing plant is coal from the mines and the output is coarse coal to the Gas Production plant and fine coal to the Steam plant. The previous statement describes the process and also the path and the sequence or direction of the flow in that part of the Synthetic Fuel plant. The process can be derived by comparing the input (singular or multiple) and the output (singular or multiple) that are indicated in Columns 4 and 5 respectively of Table A1. In the case of the Coal Processing plant the process is to separate the coal from the mines into coarse and fine coal with sieves. The path and the sequence or direction of the flow can be derived from Figure 1.2 and Table A1. The plant (or plants) from which input (singular or multiple) is received and the plant (or plants) to which output (singular or multiple) is sent are indicated in brackets in Columns 4 and 5 respectively of Table A1.

The presence of feedback-loops and the division of the output of both the Steam and Oxygen plants are of special significance. Crowe *et al.* (1971:14) refer to a feedback-loop as recycle and indicate that it is a common feature of chemical processes.

> "*Most chemical processes have recycle of either matter or heat. Recycle means that a stream leaving a process unit affects a steam entering that unit.*"

The output of Plant(II)-A progresses through Plant(II)-B and Plant(III) and eventually it ends up as the input of the Division Process plant. From the Division Process plant there is a direct feedback-loop to Plant(II)-A and there is also an indirect feedback-loop through the Recycling plant to Plant(II)-A. The output of the Steam plant is divided between three other plants. Steam is supplied to both the Gas Production and Oxygen plants, while any additional steam is sent to the Electricity Generation plant. The output of the Oxygen plant is divided between two other plants. Oxygen is supplied to both the Gas Production and Recycling plants. The ramifications of these phenomena on a simulation model are detailed in Sections 2.1, 2.2, 2.4, 2.5 and 2.7.

The process logic (rules of operation) or controls according to Harrell and Tumay (1999:1) of the Synthetic Fuel plant are presented in Appendix B: *Synthetic Fuel Plant Rules of Operation*. For example, one of the rules of operation states that steam will only be supplied to the Electricity Generation plant once the Gas Production and Oxygen plants have been supplied. The supply of steam to the Gas Production and Oxygen plants is therefore the primary function of the Steam plant while the supply of steam to the Electricity Generation plant is the secondary function of the Steam plant. These rules of operation, if complex, can have a severe impact on the complexity of a simulation model.

That concludes the description of the system that is considered in this document, according to the system description breakdown that is developed in the first paragraphs of this section.

The process flow describes the processes and also the path and the sequence or direction that the "commodities" that move of flow through the system follow. The "commodities" themselves, however, also have to be described. These "commodities" can be as diverse as data, electrical currents, entities, solids, liquids, gases, *etc.* If the "commodities" are discrete entities the motion is referred to as move and if the "commodities" are fluid in nature the motion is referred to as flow. A scrutiny of Figure 1.2 and Table A1 indicates that, in this instance, the "commodities" are coal, various gases (steam, oxygen, raw gas, pure gas, residue gas, *etc.*) and various liquids (water, gas-water, condensate and chemical products). Even though the coal from the mines is in the solid phase, it is considered as a fluid because it consists of chunks that are moved along on conveyor belts. The same logic applies to the coarse coal that is supplied to the Gas Production plant while the fine coal that is supplied to the Steam plant is in the form of a slurry (a suspension of insoluble particles). The motion of the coal, gases and liquids in the Synthetic Fuel plant is therefore characterised as flow.

Summary

The system description that is provided in this section gives an indication of the type of system that is considered in this document and also provides an insight into the level of detail that is deemed necessary if a simulation model of the system for strategic decision support is considered. The system description is used as the model definition when a simulation model of the system is developed.

* * * * *

1.3 SIMULATION MODELLING AS A DECISION SUPPORT TOOL

> "*It must be remembered that there is nothing more difficult to plan, more doubtful of success, nor more dangerous to manage, than the creation of a new system.*"
>
> Niccolò Machiavelli

This statement, made approximately 500 years ago by Machiavelli (1469 - 1527), regarding the challenge of planning and managing political systems, is equally applicable to the design and operation of modern day manufacturing systems (Harrell and Tumay, 1999:1).

Management can be described as the art of making decisions without having all the relevant information available. There is a commonly held belief that by the time all the relevant information about a decision is available, it may not be important or even necessary to make the decision any more (*i.e.* the time window of opportunity or impact of that decision has already passed). Managers would therefore like to have a "toolbox" of decision support tools available to help them to make better decisions. The goal is to decrease the risk associated with a decision and consequently to increase the confidence level that the correct decision is made. Morris (1977:1) describes a decision aid as "*... a model, method, technique, or process designed to enhance the decision-making process.*"

Figure 1.4: *Decision Support Tool Confidence Level* (adapted from Kleinschmidt (1990)) gives an indication of the confidence levels that can be obtained with different decision support tools.

The vertical axis represents the confidence level that can be obtained that the determined value of an attribute of a system is correct. The attribute that is under scrutiny can be as diverse as the performance of an aircraft or the environmental impact of a chemical plant. The confidence level that the determined value of an attribute of a system is correct can vary between 0% and 100%. The horizontal axis represents different decision support tools that can be used to obtain a required confidence level.

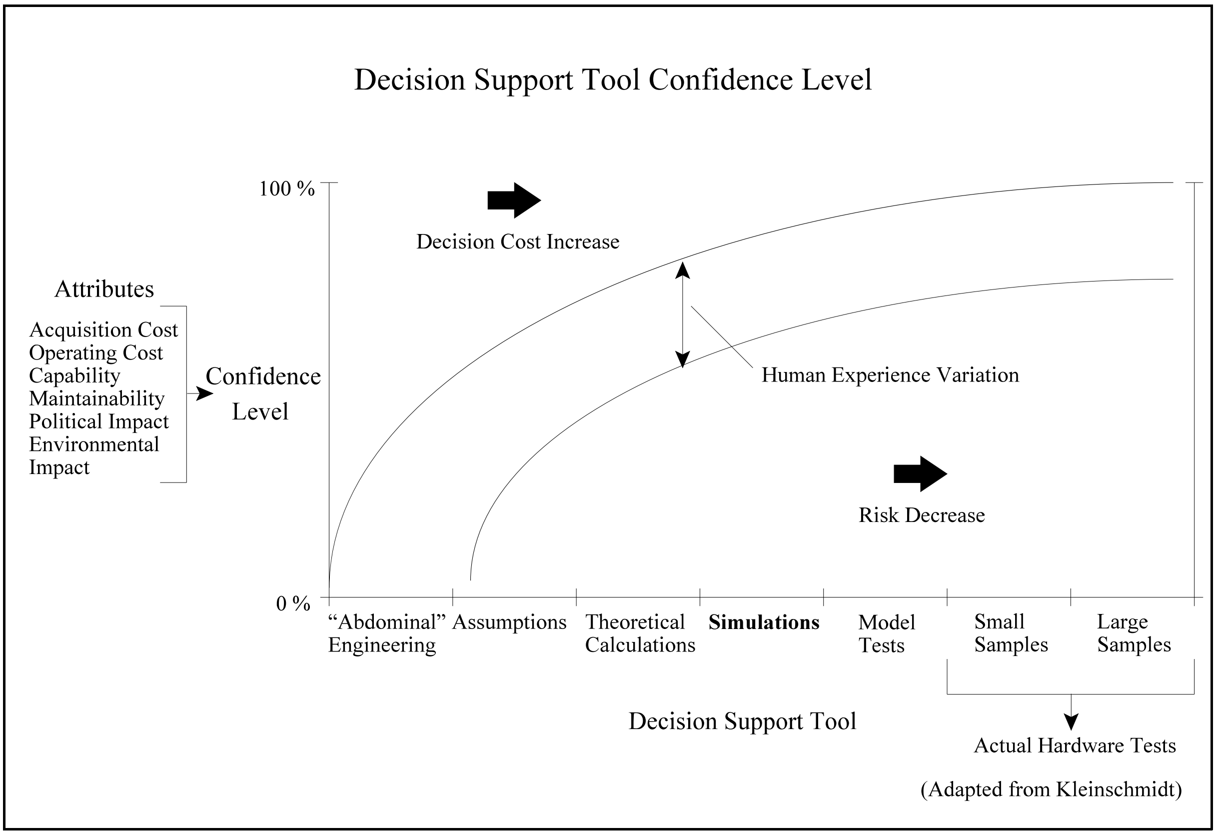


Figure 1.4: Decision Support Tool Confidence Level

"Gut feel" decisions or "abdominal" engineering features on the extreme left of the horizontal axis. This represents intuitive decisions, usually taken when there is very scant information or not enough time available to make a structured decision. Naturally the confidence level of an attribute value of a system that is determined with this decision support tool is not very high. Large samples are positioned on the extreme right of the horizontal axis. If a sample batch of a number of aircraft has been built and tested, the confidence level of the determined value of the performance attribute of the aircraft can be very high. The confidence level of an attribute value of a system that is determined with a large sample can approach 100%. There is a bandwidth of variation in the confidence level of the determined value of an attribute, depending on the experience level of the person involved. Obviously the "gut feel" decision of a very experienced person can be more accurate than the theoretical calculation of a novice in the field.

Simulations are found midway between "gut feel" decisions and large samples. Simulations are better than theoretical calculations because it generally uses stochastic methods to incorporate the effect of random events into the calculations. Theoretical calculations are usually deterministic (*i.e.* based on exact mathematical equations) and are therefore further removed from the real-world situation than simulations that can incorporate random events.

In a grey area between theoretical calculations and simulations are mathematical models (not indicated in Figure 1.4), which are sometimes considered as either a subset of theoretical calculations or simulations, depending on personal preference. Taha (1987:12-13) compares mathematical models with simulation models.

> "*Simulation models, when compared with mathematical models, do offer greater flexibility in representing complex systems. The main reason for this flexibility is that simulation views the system from a basic elemental level. Mathematical modeling* [*sic*], *on the other hand, tends to consider the system from a less detailed level of representation.*"

It is interesting to note that when Sasol Synfuels decided not to go ahead with the update of the final 1996 simulation model in 1999, they decided to develop a Linear Programming (LP) model as a decision support tool. Various handbooks on Operations Research (OR) explain the development and use of LP models, for example, Hadley (1975), Luenberger (1973:9-106) and Taha (1987:25-300). As a decision support tool an LP model is very powerful but it is limited in its range of application and some authors like Harrell and Tumay (1999:4) clearly indicate its shortcomings.

> "*Traditional methods, such as work analysis, flow charting, process mapping,* ***linear programming****, etc. are incapable of solving the complex integration problems of today. These tools have only limited application and are* ***unable*** *to provide a* ***reliable measure of expected system performance****.*" [Bold typeface added for emphasis]

Harrell and Tumay (1999:9) also indicate one of the major benefits of a simulation model that sets it apart from traditional methods such as LP programming.

> "*It also enables one to gain an overall understanding of the* ***system dynamics*** *that would otherwise be difficult to obtain.*" [Bold typeface added for emphasis]

Simulations are the last "soft" way of testing an idea before moving on to the real-world hardware of physical models and samples of the actual hardware. It can intuitively be judged that there will be an increase in the cost of decision support from left to right as one moves from "gut feel" decisions to large samples. This increase in the cost of decision support goes hand in hand with a decrease in the risk that is associated with a decision. It is therefore evident that managers pay for their peace of mind. The question is how much are managers prepared to pay for their peace of mind? It seems as if simulation is a way of buying adequate peace of mind, without paying an excessively high cost penalty by moving on to physical model and actual hardware tests.

Morris (1977:1) describes decision-making behaviour as characterised along a continuum from random decision-making behaviour at one extreme, through inspirational decision-making behaviour, to systematic decision-making behaviour at the other extreme. This corresponds strongly with the aforementioned line of reasoning. The reference also indicates that systematic decision-making behaviour is preferable.

> "*There is a strong belief, and considerable evidence to support the belief, that systematic decision making increases the probability of achieving a good outcome.*"

The path to understanding the behaviour of a system can be characterised as progressing through four different levels, namely: data, information, knowledge and insight. When the data about the behaviour of the system are processed, it leads to information about the behaviour of the system. The information about the behaviour of the system is available to the managers, but to make truly inspired decisions, the managers need knowledge about and insight into the behaviour of the system. This is the domain where simulation modelling as a decision support tool really comes into its own right. A simulation model can provide knowledge about past and present system behaviour as well as insight into probable future system behaviour (within reasonable limits). For example, a simulation model can be used to identify the "bottlenecks" that currently exist in a system, thus providing knowledge about past and present system behaviour. The simulation model can alternatively also be used to predict system behaviour for different proposed strategies to alleviate the "bottlenecks", thus providing insight into probable future system behaviour. This is comparable to the view of Harrell and Tumay (1999:5) about the role of simulation modelling.

> "*Simulation itself does not solve problems, but it does clearly identify problems* [provides knowledge about past and present behaviour] *and quantitatively evaluate alternative solutions* [provides insight into future behaviour]."

It seems as if managers are becoming progressively more aware of the power of simulation modelling as a decision support tool. Owen (1994:15,17) indicates that large chemical plants are making extensive use of modelling and simulation.

> "*... manager engineering, believes it is essential for large industrial companies to develop and implement a strategic approach to corporate maintenance philosophy and programmes to sustain competitive advantage.*"

> "*... uses sophisticated, computerised optimisation technology to assist with the more complex needs.*
>
> *These computerised techniques include ...* [various other techniques] *... and complete plant modelling and simulation.*"

The objective is to achieve the maximum possible rate of production and consequently also the maximum possible profitability. The manual of Extend™ (2000:E14) describes a common goal of business.

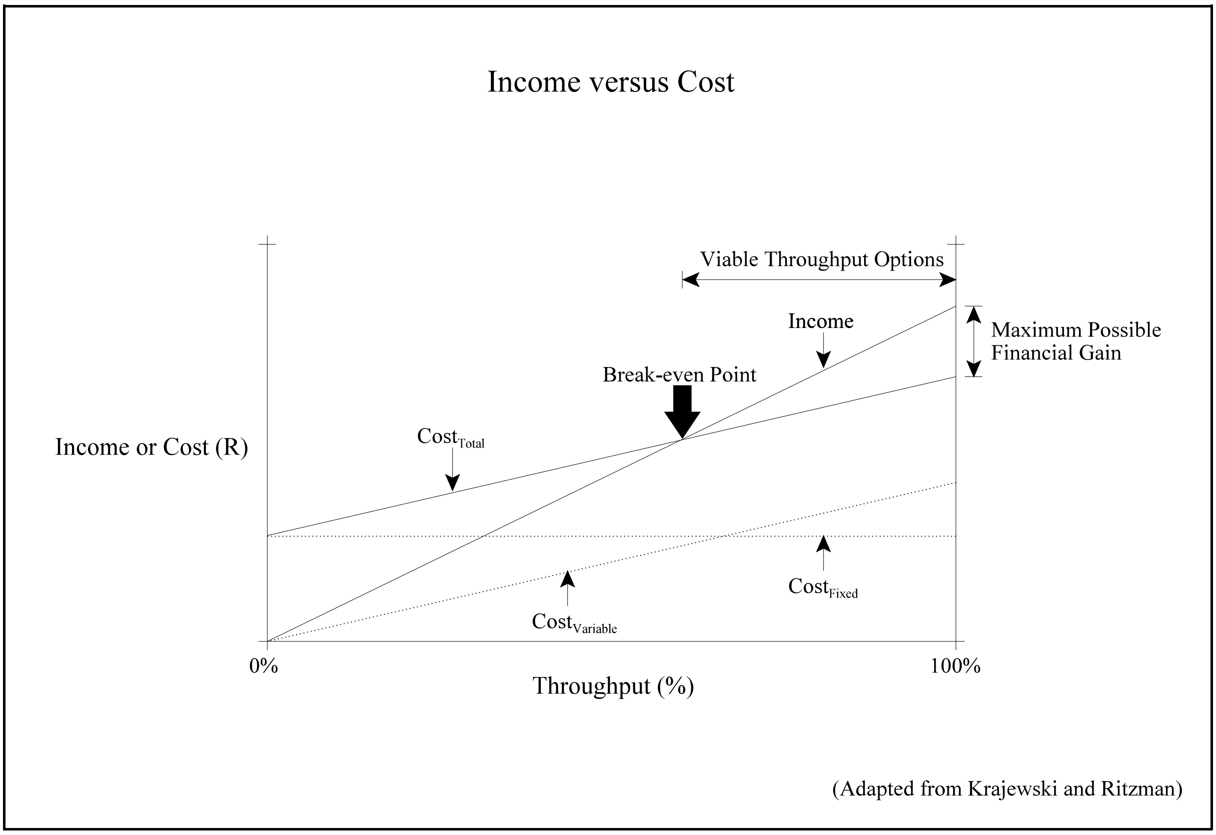
> "*In business, a common goal is to optimize a system such that it processes the most things using the least amount of resources and time.*"

From the first principles of economics it follows that the total cost of production can be divided into the fixed cost and the variable cost (Lipsey and Harbury, 1988:167).

$$Cost_{Total} = Cost_{Fixed} + Cost_{Variable} \quad (monetary\ unit) \qquad (Eq.:1.1)$$

The total cost of production is the cost of production at any given rate of production or throughput. Fixed cost does not vary with variation in the throughput while variable cost varies with variation in the throughput. Variable cost usually increases linearly with an increase in the throughput (*i.e.* variable cost is usually directly proportional to the throughput). This concept is graphically depicted in Figure 1.5: *Income versus Cost* (adapted from an example in Krajewski and Ritzman (1990:48)).

Income also usually increases linearly with an increase in the throughput (*i.e.* income is usually directly proportional to the throughput). From the first principles of economics it follows that the financial gain (profit) is the income minus the total cost.



(Adapted from Krajewski and Ritzman)

Figure 1.5: Income versus Cost

$$Gain_{Financial} = Income - Cost_{Total} \quad (monetary\ unit) \qquad (Eq.:1.2)$$

From Figure 1.5 it follows that the only viable throughput options are those that achieve better results than the one that achieves break-even results. The maximum possible financial gain is achieved with 100% throughput. The managers of a plant will therefore always strive towards maximisation of the throughput. (This assumption is only valid if it is assumed that there is an infinite market for the throughput of the plant, or at least “infinite” up to 100% of the throughput of the plant.) The aforementioned argument correlates closely with the optimisation principle that is supplied by Morris (1977:14).

> “*We would like to maximize some function of the benefits and costs, say the difference between benefit and cost, or the ratio of benefit to cost.*”

Taha (1987:5) advocates that a decision support model must include the following elements:

a) Decision alternatives (probable scenarios) from which a selection is made.
b) Restrictions for excluding infeasible alternatives.

c) Criteria for evaluating and ranking alternatives.

All throughput options that achieve worse results than the one that achieves break-even results can be considered as infeasible alternatives (see Figure 1.5). In this instance the financial gain that is realised by each alternative is the criterion for evaluating and ranking alternatives.

Douglas (1972:7) supports this view in his discussion about the optimal control of process dynamics.

> "*Optimal control problems in the chemical and petroleum industries are similar to the preceding ones with the exception that the possibility of using profit as the performance criterion we wish to maximize must also be considered.*"

Summary

This section indicates how simulation modelling reduces the risk that is associated with decisions. Managers need decision support tools to achieve the maximum possible rate of production or throughput and consequently also the maximum possible profitability. Simulation modelling is a cost-effective way of attaining a high level of confidence in a decision. It is a low risk and a low cost decision support tool that managers can use to help them in the process of making better decisions. Harrell and Tumay (1999:9) provide a good synopsis of the role of simulation modelling in decision support.

> "*The key to sound management decisions lies in the ability to accurately predict the outcome of alternative courses of action. Simulation provides precisely that clarity of foresight.*"

* * * * *

1.4 SHORTCOMINGS OF THE ORIGINAL METHOD

The first section of this chapter refers to the original simulation model of the Sasol East plant that was developed from 1994 to 1996. The development of the original simulation model is the subject matter of a *Magister* dissertation (Albertyn, 1995). This section provides a very basic introduction to the original simulation model and details the shortcomings of the original simulation modelling method. The following abstract from a published article provides a short overview of the dissertation (Albertyn and Kruger, 1998:1):

> "*The key objective is to develop a method which can be utilised to model a stochastic continuous system. A system from the "real world" is used as the basis for the simulation modelling technique that is presented. The conceptualisation phase indicates that the model has to incorporate stochastic and deterministic elements. A method is developed that utilises the discrete simulation ability of a stochastic package (SIMAN), in conjunction with a deterministic package (FORTRAN), to model the continuous system. (Software packages tend to specialise in either stochastic or deterministic modelling.) The length of the iteration time interval is investigated and different methods are investigated and evaluated for the determination of adequate sample size. The method is authenticated with the verification and validation of the defined model. Two scenarios are modelled and the results are discussed. Conclusions are presented and strengths, weaknesses and further developments of this method are considered and discussed.*"

In the dissertation the original simulation model is used to identify the problem areas in the plant and to study the effect of a proposed change on the plant. The first scenario identifies the "bottlenecks" in the plant and the second scenario studies the effect of an extra oxygen "train" on the plant. Both the scenarios obviously use a *circa* 1995 system description or model definition of the plant. The first scenario thus provides knowledge about the then "past" and "present" behaviour of the plant and the second scenario provides insight into the then "future" behaviour of the plant. The addition of an extra oxygen "train" was chosen as a scenario because it was one of the real-world decision options that confronted the management of the plant at that time. The position of the extra oxygen "train" is indicated in Figure 1.2, the number of modules and their input and output capacities are indicated in Table A1 and the service schedules and failure characteristics of the modules are indicated in Table A2.

The original simulation model was developed in the SIMAN environment and it incorporates a Microsoft FORTRAN subroutine. SIMAN is a simulation software package from the now defunct Systems Modeling Corporation and Microsoft FORTRAN is a general scientific and engineering software package from the Microsoft Corporation. SIMAN has since been superseded by Arena. Arena is a simulation software package that started its life with the Systems Modeling Corporation but now forms part of the Rockwell Software Incorporated suite of software products. The original simulation model of the Sasol East plant was subject to further development, refinement, expansion and maintenance over the latter part of the 3-year time period from 1994 to 1996. During this process the final 1996 simulation model (that included the whole Sasol Synfuels complex) was upgraded to one of the first versions of Arena and it incorporates a WATCOM FORTRAN subroutine. WATCOM FORTRAN is a product of the WATCOM International Corporation.

SIMAN, Microsoft and Arena are registered trademarks and are usually denoted by SIMAN®, Microsoft® and Arena® respectively. However, for the sake of simplicity they will be written simply as SIMAN, Microsoft and Arena in this document. The same logic applies to WATCOM which is a trademark and usually denoted by WATCOM™.

The reasons why a FORTRAN subroutine was included into the original simulation model should be clear from the following quotation indicating the strengths of the original simulation modelling method, as detailed in the dissertation (Albertyn, 1995:106-107):

> "***Strengths of the method***
>
> ...
>
> *i)* *The method allows the modeller to incorporate complex decision-making processes into the model by virtue of the inclusion of FORTRAN. (The complex logic calculations associated with the determination of the number of modules to be switched on or off and the throughput, can readily be handled by FORTRAN, because it is a computer language designed for complex mathematical calculations.)* [The momentary "bottleneck" is also identified by the FORTRAN subroutine.]
>
> *j)* *FORTRAN poses virtually no restriction on the number of variables that can be addressed in the FORTRAN subroutine.*
>
> *k)* *Additional output files can be generated with ease from within the FORTRAN subroutine. (It allows the modeller more flexibility in terms of*

information that can be made available.)

l) *"User-friendliness" is enhanced by the use of input files, because the input files allow the modeller to implement certain changes fast and without much effort.*

...

n) *The incorporation of FORTRAN into the model to handle the complex mathematical calculations that are required assists in keeping simulation runtimes within acceptable limits. (FORTRAN is ideally suited to handle complex mathematical calculations in a fast and efficient way, whilst SIMAN would be slow and cumbersome if it were utilised to deal with the same calculations.)*"

The most important benefits of using a FORTRAN subroutine are the arguments that are stated under Points i) and n). The FORTRAN subroutine allows complex decision-making processes (*i.e.* the rules of operation of the plant) to be incorporated into the simulation model and it also helps to keep simulation runtimes within acceptable limits.

The weaknesses of the original simulation modelling method are also detailed in the dissertation (Albertyn, 1995:108) and they are presented in the following quotation:

"***Weaknesses of the method***

a) *The fact that SIMAN does not have a sufficiently well developed graphics capability makes for more difficult debugging and also impacts adversely on client acceptance of the model.*

b) *The inherent SIMAN restriction on the number of variables that can be addressed hampers model conceptualisation and development. (It sometimes forces the modeller to revert to less elegant modelling techniques.)*

c) *The FORTRAN subroutine has extremely complex structures and to a large extent it is not generic. (In fact, a small change in the model definition or conceptualisation can possibly lead to major changes in the FORTRAN subroutine.)*

d) *The method gives rise to a very complicated structure, involving two different software packages and complex interfacing, compiling and linking.*

> e) *The complex structure of the model complicates debugging. (It is sometimes difficult to assess whether a faulty event occurs in the SIMAN model, or in the FORTRAN subroutine.)*
>
> f) *The stochastic nature of the model also complicates debugging. (Even though the modeller may provide for all possible combinations and permutations of feasible events, the stochastic nature of the model will result in the code not necessarily following a specific logic loop, until a certain sequence of events has taken place.)*"

The following exposition provides more detail about the weaknesses of the original simulation modelling method. The arguments of Points a) and b) are not valid anymore since SIMAN has been superseded by Arena. Arena has a good graphics capability and virtually no realistically achievable restriction on the number of variables that can be addressed. The arguments of Points c), d) and e) are the main concerns. The argument of Point f) is a universal problem that is characteristic of all stochastic simulation models.

Point c) of the weaknesses indicates that the FORTRAN subroutine has a complex structure and to a large extent it is not generic. This may lead to difficulty when changes in the system description or model definition of the plant need to be accommodated. The system description (see Section 1.2) of the plant is representative of the real plant and it is not static. The system description evolves over time as new chemical processes are introduced to increase efficiency and to align product supply with product demand.

The original simulation modelling method can easily accommodate the following changes in the system description of the plant through the manipulation of the input files:

a) Changes in the number of modules in each of the smaller plants.
b) Changes in the input and output capacities of the modules.
c) Changes in the service schedules of the modules (*i.e.* the start times, cycle times and service times of the service cycles).
d) Changes in the failure characteristics of the modules (*i.e.* the failure rates and repair times).
e) The inclusion or exclusion of the extra oxygen "train".

However, the original simulation modelling method has difficulty in accommodating changes in the system description of the plant that concern the configuration, process flow or process logic. For example, if the plant configuration is changed by the addition of another smaller plant, it cannot be accommodated by merely manipulating the input files. This is also true if the process flow or process logic is changed. For example, if feedback-loops are changed (*i.e.* moved, removed or added) or if the rules of operation of the plant are changed, it cannot be accommodated by the manipulation of the input files. None of the aforementioned changes can be accommodated without substantial changes in the FORTRAN subroutine.

Point d) of the weaknesses indicates that the original simulation modelling method leads to a complicated structure with two different software packages and therefore complex interfacing, compiling and linking. The whole process is time-consuming and it is easy to lose track of what is going on (Albertyn, 1995:58-63). The structure is much simpler if the whole simulation model resides as a single simulation model (without a subroutine) in one simulation software package. In such an instance there is no interfacing between different software packages and usually less complex compiling and linking.

Point e) of the weaknesses indicates that the complex structure of the original simulation model complicates "debugging" because it is sometimes difficult to determine whether a faulty event occurs in the SIMAN part of the original simulation model or in the FORTRAN subroutine. Once again it can intuitively be judged that "debugging" is easier if the whole simulation model resides as a single simulation model (without a subroutine) in one simulation software package.

Point f) of the weaknesses indicates that the inclusion of random behaviour complicates "debugging". Unfortunately it is an inherent problem of all stochastic simulation models.

The following two techniques can be used to counter this problem:

a) Construct a small separate test simulation model that represents the required sequence of events to test the functioning of the specific logic loop that is under scrutiny. The disadvantage of this method is that it is time-consuming because once the test simulation model has been verified and validated, the code must be transferred into the real simulation model.

b) Force the simulation model with external input to generate the required sequence of events to test the functioning of the specific logic loop that is under scrutiny. This is also time-consuming because the state of the simulation model at any given time is defined by a "state vector" that comprises all the variables of the simulation model. In order to force the process logic of the simulation model to consider a specific logic loop, input values that lead to that specific logic loop have to be supplied for every variable in the "state vector" (simulation model).

Summary

This section explains why a FORTRAN subroutine was included into the original simulation model and details the shortcomings of the original simulation modelling method. These shortcomings were the catalysts that initiated the development of the generic simulation modelling methodology that is presented in this document.

* * * * *

1.5 OBJECTIVE STATEMENT

Section 1.1 indicates that the 1999 investigation into the viability to update the final 1996 simulation model of the Sasol Synfuels complex concluded that comprehensive changes were needed. The reasons why the necessary changes cannot readily be accommodated by the original simulation modelling method are detailed in the previous section. The comprehensive changes that were needed and the inability of the original method to accommodate these changes easily, clearly indicated that there was substantial scope for further research in this area. From the outset it was envisioned that the research presented an opportunity to accomplish something more than just to solve the problem of how to accommodate the comprehensive changes that were needed for the update of the final 1996 simulation model. The research presented an opportunity to develop a generic simulation modelling methodology for a whole specific class or type of system. All systems that exhibit the same characteristics as the Sasol East plant can readily be accommodated by the generic methodology. These characteristics and their implications are discussed in detail in Sections 2.1 and 2.2. Systems of this class or type of system are described as stochastic continuous systems, thereby referring to their two most distinctive characteristics, namely: they are subject to random (stochastic) phenomena such as failures and characterised by continuous processes (flow).

The key objective of this research is to develop a generic simulation modelling methodology that can be used to model stochastic continuous systems effectively.

The generic simulation modelling methodology is able to accommodate any generic variant of a stochastic continuous system of approximately the same size and complexity, and to the same level of detail, as the system that is detailed by the system description in Section 1.2 (*i.e.* the Synthetic Fuel plant that represents the Sasol East plant). Of course, the generic methodology can also easily accommodate any combination of stochastic continuous systems and the interrelationships between them (*i.e.* the whole Sasol Synfuels complex). The generic methodology renders simulation models that can be used as decision support tools on a strategic level of decision support (see Section 1.1).

The reasons why the generic simulation modelling methodology is effective can be attributed to a structured approach and the characteristics that are exhibited by simulation models that are developed with the generic methodology. The characteristics of the simulation models follow directly from the design criteria of the generic methodology. The design criteria are a combination of general best practise simulation modelling method design criteria and design criteria that originate from the shortcomings of the original simulation modelling method.

The characteristics (or alternatively the design criteria) of simulation models that are developed with the generic simulation modelling methodology, are the following:

a) Short development time.
b) Short maintenance times.
c) User-friendliness as perceived from the development, maintenance and usage perspectives.
d) Short simulation runtimes.
e) Compact simulation model size.
f) Robust modelling ability.
g) Accurate modelling ability.
h) Single software application.

The following points, on a one-to-one basis, provide more detail about the aforementioned characteristics of simulation models that are developed with the generic simulation modelling methodology:

a) Section 1.1 indicates that the process to bring the final 1996 simulation model to fruition took approximately three years. This is not unusual for a technically sophisticated problem (Crowe *et al.*, 1971:5). A longer development time implies that larger resources of manpower and money must be committed from the outset to ensure probable success. It is also sometimes difficult to keep up enthusiasm for the project over a longer time span. Management always “needs the answer now”. A shorter development time implies that fewer resources are needed as well as more enthusiasm and easier attainment of permission from management to proceed with the project.

b) The previous section indicates that the original simulation modelling method placed severe restrictions on the speedy implementation of comprehensive changes to the final 1996 simulation model. The same arguments as stated in the previous point are also valid in this instance and therefore it is obvious that great benefit can be derived if maintenance times are shorter.

c) User-friendliness is a very important aspect of simulation models as far as acceptance and continued use are concerned (Bonnet, 1991:12-13).

> "*Even though less and less* [*sic*] *people are still intimidated by a computer and the actual answers of a simulation are what is of importance, user-friendliness still (unconsciously or otherwise) promotes the use of a program.*"

The user-friendliness of the original simulation modelling method is listed as a strength because input files are used to manipulate the simulation model (Albertyn, 1995:107). Input files or spreadsheets greatly enhance the user-friendliness of simulation models. The use of graphics and animation can also benefit user-friendliness and help with simulation model "debugging" (Elder, 1992:3-4,72,277; Pegden *et al.*, 1990:305-308). Pegden *et al.* (1990:308) describe some of the benefits of animation.

> "*The animation also played an important role in model verification and validation. ... Consequently, management had high confidence in the model.*"

There is a trend among the managers that use simulation modelling as a decision support tool to get more directly involved in the simulation modelling process. They do not only want the answers to a few preselected questions anymore. They want access to decision support on a continual basis. This implies a requirement for user-friendly simulation models that can be used directly by the managers themselves or by the industrial engineers that support them. Consequently the use of graphics and animation is becoming increasingly important. The results of a survey that probed the importance of graphics and animation in simulation models, as compared to purely statistical models, indicate the importance of graphics and animation. The majority of the respondents (81%) rated graphics and animation as "very important" (36%) or "important" (45%). Only a small percentage (19%) of the respondents rated graphics and animation as "somewhat important" (Simulation Fax Survey Results, 1993:10). Bonnet (1991:13) indicates that user-friendliness is even more important if the simulation model is going to be used by someone else than the person who developed it.

> "*In conclusion, if the program is to be used only by the programmer, user-friendliness is very often not worth the trouble, since the programmer knows the program inside out. If the simulation is intended to be used by others, such as in this case, user-friendliness is an* ***essential prerequisite****.*"
> [Bold typeface added for emphasis]

d) Short simulation runtimes for simulation models help to keep the development and maintenance times within acceptable limits. It is also advantageous during sensitivity analysis or scenario analysis.

e) A compact simulation model size enhances the transportability of simulation models between different computers and over the Internet and it is an advantage when simulation models are stored on magnetic media. There is also an indirect advantage during the development and maintenance of simulation models, because it is easier to keep track of "what" is being done "where" in structured, compact simulation models than in less structured, dispersed simulation models.

f) In this instance a robust modelling ability refers to the capacity of the generic simulation modelling methodology to facilitate the accommodation of any generic variant of a stochastic continuous system. It also indicates that comprehensive changes to simulation models can easily be handled by the generic methodology.

g) The generic simulation modelling methodology renders simulation models that are very accurate when compared to acceptable industry standards. Accuracy is not compromised for the sake of any of the other characteristics or design criteria.

h) The previous section clearly indicates the difficulties (*i.e.* the complex structure and difficult interfacing, compiling and linking) associated with a simulation modelling method that uses two different software packages to construct a simulation model. The generic simulation modelling methodology is structured to accommodate a simulation model in one simulation software package and therefore avoids these pitfalls.

Summary

To summarise this section, the key objective of this document is to present a generic simulation modelling methodology. The generic methodology can be used to model any generic variant of a stochastic continuous system. Simulation models that are developed with the generic methodology exhibit the following characteristics: short development and maintenance times, user-friendliness, short simulation runtimes, compact size, robustness, accuracy and a single software application.

* * * * *

1.6 IMPORTANCE OF THE RESEARCH

Section 1.1 indicates that the comprehensive changes that were needed in 1999 to update the final 1996 simulation model of the Sasol Synfuels complex necessitated the proposal of a lengthy and therefore costly process. This can be ascribed to the shortcomings of the original simulation modelling method (see Section 1.4). The discussion of the characteristics of the generic simulation modelling methodology in the previous section indicates that the generic methodology successfully nullifies, circumvents or lessens the impact of the shortcomings of the original method. It can therefore be assumed that the project might have proceeded in 1999 if the generic methodology was available at that time.

Even though Sasol claims that the Sasol Synfuels complex is the only commercial coal-based synthetic fuel manufacturing facility in the world, an article in *Encyclopaedia Britannica* (2002) indicates that a similar plant exists in Japan. Omuta, Fukuoka Prefecture, Japan has been an important industrial city since 1917. The city is situated in a coal-mining area and is especially known for the manufacture of chemicals. Coke and synthetic petroleum are listed as commodities that are produced in Omuta. (Coke is the solid substance that is left after the gases have been extracted from coal.) It is obvious that a plant that manufactures coke and synthetic fuel is very similar to the Sasol Synfuels complex and therefore the generic simulation modelling methodology can also be used to easily construct a simulation model of such a plant.

From 1994 to 1995 a simulation model of a similar plant was developed by the same company that was responsible for the development of the final 1996 simulation model. The Kynoch plant at Modderfontein, South Africa is much smaller than the Sasol Synfuels complex but it uses basically the same processes. It also uses steam and oxygen to gasify coal and then extract chemical products from the gases. In the case of the Kynoch plant the main focus is on the production of ammonia from coal. Ammonia is one of the key ingredients of fertilisers. The two simulation models (the final 1996 simulation model and the Kynoch plant simulation model) were developed in parallel by two different project teams. The Kynoch plant simulation model is much simpler than the final 1996 simulation model and does not use the same simulation modelling method. For example, the Kynoch plant simulation model only evaluates three points in the plant for the identification of the momentary "bottleneck", while the final 1996 simulation model evaluates 13 points in each of the Sasol East and Sasol West plants for the identification of their respective momentary "bottlenecks". The simulation modelling method that is used in the Kynoch plant simulation model, however, does not render very good results, because the system description or model definition of the plant was appreciably simplified to enable the entire simulation model to be accommodated in Arena. The project team of the Kynoch plant simulation model did not want to include a FORTRAN subroutine to handle the complex aspects of the simulation model. It stands to reason that the original simulation modelling method that was used for the final 1996 simulation model could also have been used for the Kynoch plant simulation model because of the degree of commonality between the Kynoch plant and the Sasol East and Sasol West plants. It can therefore be concluded that the Kynoch plant is also an excellent candidate for a system that could benefit tremendously from the advantages that are rendered by the generic simulation modelling methodology.

There are many crude oil refineries all over the world that exhibit the same characteristics as the Sasol Synfuels complex and the Kynoch plant. In the case of crude oil refineries the input of the process is crude oil rather than coal but in all other aspects the crude oil refineries are generic variants of the system that is detailed by the system description in Section 1.2 (*i.e.* the Synthetic Fuel plant that represents the Sasol East plant). It therefore stands to reason that the generic simulation modelling methodology can be used to great advantage when simulation models of crude oil refineries are required.

The Sasol Synfuels complex represents the oil-from-coal process but an equally important aspect which has developed recently is the gas-to-liquids (GTL) process. The following quotation provides some background on the subject (Sasol: Technologies & Processes, 2003):

> "*The Sasol Slurry Phase reactor at Sasolburg has been attracting international interest because of the world's abundant natural gas reserves and the mounting environmental lobby for cleaner burning fuels. The Slurry Phase reactor is at the heart of the tree-step SPD* [Slurry Phase Distillate] *process, which converts natural gas into high-quality low-emission diesel. The SPD diesel is more environmentally benign than the developed world's current and proposed generations of reformulated diesels.*"

Sasol is involved in GTL projects in South Africa, Qatar, Nigeria and Mozambique (Heckl, 2003:2; Fraser, 2002:1,14; Sasol's natural gas project surging ahead in Mozambique, 2002:7). Sasol expects its GTL investments to be producing five hundred thousand barrels of diesel a day in 10 years time (Fraser, 2002:1). Even though Sasol is considered as one of the leaders in this technology field, there are many other companies that are equally interested and active in the GTL environment. According to Bridge (2004:15) the PetroSA plant at Mossel Bay, South Africa is the largest commercial GTL plant in the world. (PetroSA was formed through the merger of Mossgas and Soekor in 2001.) Naturally, any GTL plant simulation model can easily be developed by applying the generic simulation modelling methodology.

The previous paragraphs clearly indicate the possible range of application of the generic simulation modelling methodology in the petrochemical industry. The oil-from-coal process, the classic crude oil refinement process and the GTL process can all be accommodated by the generic methodology without any difficulty. However, the possible range of application of the generic methodology is not restricted to the petrochemical industry. Any plant that exhibits the same characteristics as the Sasol East plant can readily be accommodated by the generic methodology. For example, a plant that manufactures paints obviously falls within this class or type of system. It thus stands to reason that the generic methodology can also be used to develop a simulation model of such a plant without great effort.

Traditionally the development of simulation software packages has focused primarily on the ability to model discrete-event systems. Harrell and Tumay (1999:34) indicate that this trend can be explained by the fact that most manufacturing and service systems are discrete-event systems. This leads to the phenomenon that most simulation software packages cannot adequately accommodate continuous systems. For example, Harrell and Tumay (1999) dedicate only approximately 3% of their book to the modelling of continuous systems (two pages to theory and seven pages to applications out of a total of 309 pages). Kelton *et al.* (1998) fare even worse and dedicate less than ½% of their book to the modelling of continuous systems (two pages out of a total of 547 pages). Pegden *et al.* (1998) dedicate a whole chapter to the modelling of continuous systems but this is still less than 6% of their book (33 pages out of a total of 600 pages). The *Simul8®: Manual and Simulation Guide* (1999) does not even address continuous systems. The closest reference to continuous systems is a description of batch modelling techniques that can be used for high volume applications like Business Process Re-engineering (BPR) and Fast-moving Consumer Goods (FMCG) applications.

Some authors propose that it is sometimes possible to model continuous phenomena using discrete-event modelling techniques (Harrell and Tumay, 1999:35; Kelton *et al.*, 1998:353).

Harrell and Tumay (1999:35) suggest the following technique as the first of two possible techniques that use discrete-event modelling techniques to deal with continuous phenomena:

> "*Often it is possible to model continuous phenomena using discrete-event logic, especially* ***if a high degree of precision is not important****. For example, continuous flowing substances such as liquids or granules can be converted, for purposes of simulation, into discrete units of measure such as gallons or pounds.*"
> [Bold typeface added for emphasis]

This technique can only be used if accuracy is not of paramount importance. It is therefore evident that this technique cannot be used by the generic simulation modelling methodology, as it clearly violates the design criterion that identifies accuracy as one of the required characteristics of simulation models that are developed with the generic methodology (see Point g) of the design criteria in Section 1.5). (Obviously this technique was also not used by the original simulation modelling method.)

Harrell and Tumay (1999:35) then proceed by indicating the second of two possible techniques that use discrete-event modelling techniques to deal with continuous phenomena.

> "*Another method is to simply update a variable at regular time intervals that accounts for a constant rate of change that occurred over the interval.*"

It is important to note that both the original simulation modelling method and the generic simulation modelling methodology use this technique (or a variation thereof) to determine the pertinent values of continuous phenomena as exact real numbers, thereby achieving very high accuracy. For example, the *Magister* dissertation (Albertyn, 1995:76) indicates that the original simulation model deviates less than 1% (0,59%) from the real-world situation for a known scenario. This technique is referred to as the variables technique and it is detailed in Sections 2.2 and 2.7.

The continuous modelling ability of Arena is described in its manual (Arena, 1998:145-148). Closer examination reveals that this modelling ability consists of the modelling of a container. It allows the modelling of the level and rate of change of a container that can be one of three possible types: a source, a transfer or a sink container. Containers or tanks are usually used as storage devices in continuous systems at the beginning (source containers) or the end (sink containers) of processes. Intermediate containers or tanks (transfer containers) are usually used to buffer or dampen oscillations in the system that may result because of sudden changes in production capacity that are caused by services and failures. For example, a container or tank can be used to absorb the upstream production that cannot be processed by the "bottleneck" plant, until the "bottleneck" plant is restored to adequate capacity. This concept is more applicable to liquids than gases. In most cases it is impractical to store huge volumes of gases in containers or tanks (especially if the processes that are involved are temperature and pressure sensitive). For example, in the Synthetic Fuel plant there are no tanks in the part of the process where the products are in the gas phase. The only tank in the plant is situated directly in front of Plant(IV) where it is used to buffer the flow of gas-water (in the liquid phase) between the Temperature Regulation plant and Plant(IV). The tank is not indicated in Figure 1.2 for the sake of simplicity and because it is considered to be an integral part of Plant(IV). The minimum and maximum allowable volumes of gas-water in the tank are indicated in Columns 4 and 5 respectively of Table A1. It is obvious that the container modelling ability of Arena can only be used for a minuscule part (*i.e.* the single instance of a tank) of the simulation model if a simulation model of the Synthetic Fuel plant is developed.

Summary

This section indicates that the generic simulation modelling methodology has a huge range of possible application in the petrochemical industry, but it is by no means restricted to only the petrochemical industry. Any system that displays the same characteristics as the system that is detailed in the system description in Section 1.2 can readily be accommodated by the generic methodology. The majority of simulation software packages cannot accommodate such systems easily because they were originally developed with discrete-event systems in mind.

* * * * *

1.7 LIMITATIONS OF THE GENERIC METHODOLOGY

Section 1.5 indicates that the systems that are considered in this document belong to a specific class or type of system. These systems are referred to as stochastic continuous systems to clearly identify their two most distinctive characteristics. Section 1.2 provides some detail about the stochastic characteristic while this section focuses on the continuous characteristic of stochastic continuous systems.

It might be prudent to start off this section with an elementary introduction into the classification of simulation models. This is necessary to classify, and to provide a specific context for, simulation models that are developed with the generic simulation modelling methodology.

According to Kelton *et al.* (1998:9) a useful way to classify simulation models is along the following three dimensions:
a) Static versus Dynamic.
b) Discrete versus Continuous.
c) Deterministic versus Stochastic.

The first dimension relates to the time period that is addressed by a simulation model. A simulation model that describes the behaviour of a system at a single point in time is called a static simulation model, while a simulation model that describes the behaviour of a system over a period of time is called a dynamic simulation model. This is analogous to a photograph (static) versus a movie (dynamic).

The second dimension relates to the way that a simulation model addresses the changes in the state of a system. The behaviour of a system over a period of time is usually characterised by changes in the state of the system. In a discrete simulation model the changes in the state of the system occur only at isolated (specific) points in time while in a continuous simulation model the changes in the state of the system occur continuously over time. A continuous simulation model usually uses algebraic, differential or difference equations to calculate the changes in the state of the system (Pegden *et al.*, 1995:6). Figure 1.6: *Discrete versus Continuous State Change* indicates the difference between a change in the state of the system at an isolated point in time and a continuous change in the state of the system that happens over a period of time.

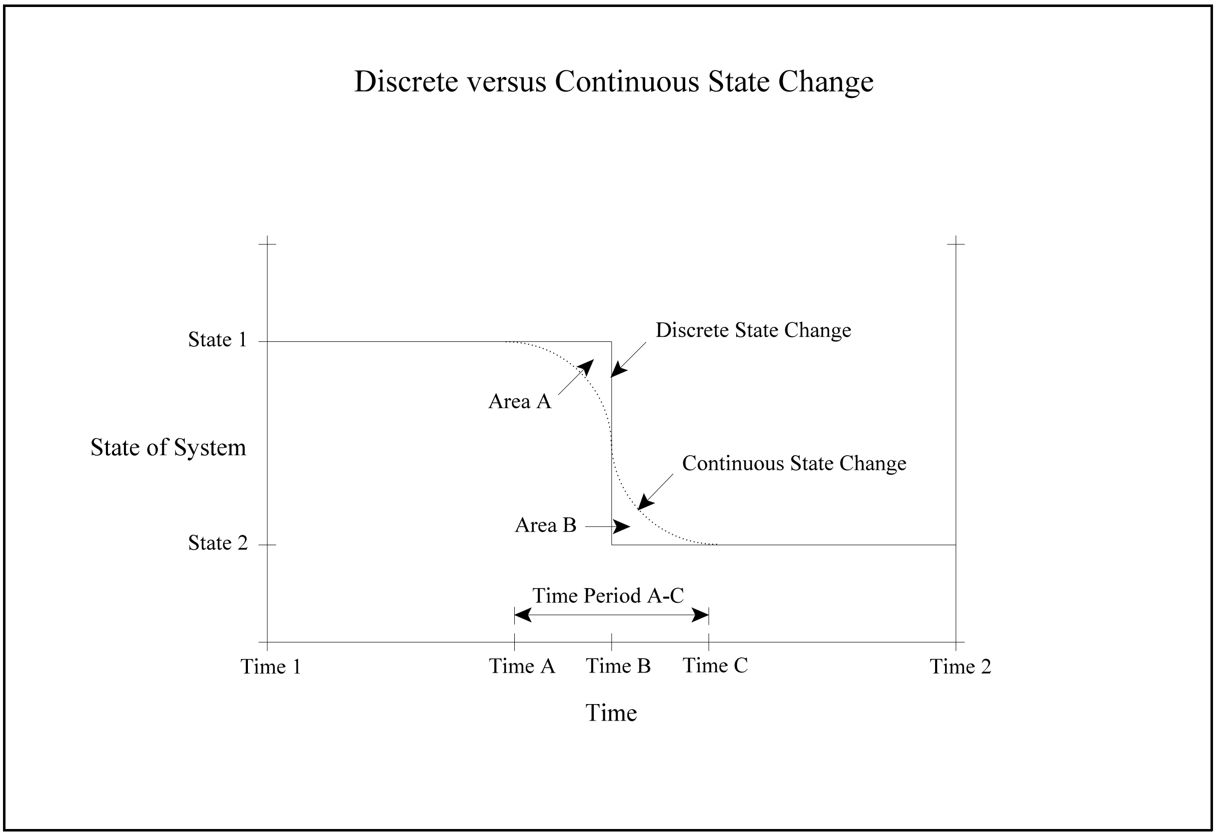


Figure 1.6: Discrete versus Continuous State Change

In Figure 1.6 a discrete change in the state of the system is represented by the solid line and it occurs at an isolated (specific) point in time (Time B) while a continuous change in the state of the system is represented by the dotted line and it occurs over a period of time (Time Period A-C). Some systems exhibit both discrete and continuous state change behaviour. Simulation models of such systems are referred to as combined simulation models. It is obvious that the Synthetic Fuel plant that is described in Section 1.2 falls within this category. The plant is characterised by a continuous process and it is also subject to discrete events, like services and failures, that cause changes in the state of the plant. Kelton *et al.* (1998:9) specifically refer to refineries as examples of combined simulation models.

The final dimension indicates whether a simulation model makes provision for random variation in the system. According to Pegden *et al.* (1995:6) very few real-world systems are free from the influence of random variation. Deterministic simulation models ignore this randomness while stochastic simulation models make provision to accommodate the randomness of the system. The Synthetic Fuel plant displays random behaviour because of the failures of the modules.

From the exposition in the previous paragraphs, it follows that it is possible to classify a simulation model of the Synthetic Fuel plant as a dynamic, combined, stochastic simulation model. The simulation model describes the behaviour of the plant over a period of time, incorporates the continuous processes of the plant, accommodates discrete events like services and failures and makes provision for the randomness of the failures.

The classification of the simulation model as a dynamic, combined, stochastic simulation model should not be confused with the description of the class or type of system that is modelled. The class or type of system that is modelled is referred to as stochastic continuous systems to emphasise the most important characteristics of the systems.

The behaviour that is exhibited when the changes in the state of the system occur continuously over time is sometimes referred to as transient behaviour (see the behaviour of the Continuous State Change over Time Period A-C of Figure 1.6). Pegden *et al.* (1995:431-464) indicate that transient behaviour is usually represented with algebraic, differential or difference equations that describe the behaviour of the system in terms of states and rates. A state equation is a direct representation that describes the state of a variable over time as an algebraic equation. In most instances it is impossible to develop a direct representation of a variable, but it is possible to establish a relationship for the rate of change of the variable with respect to time. This is an indirect representation of the variable and it is known as a differential equation. The variables that describe the state of the system can therefore be described directly by means of state equations, or indirectly by means of differential equations. The behaviour of the system is obtained by solving the state and differential equations over time. State equations are usually easy to solve mathematically. Differential equations, by comparison, are very difficult to solve mathematically and elegant mathematical solutions are available for only a few rather simplistic differential equations. In the instances where mathematical solutions for differential equations are not available, numerical techniques (known as numerical integration) are used to obtain approximate numerical values for the state of the system over time. If a simulation model contains differential equations the simulation model cannot simply jump in time between events, but is advanced in time by a series of small time intervals between the normal discrete events (assuming that it is a combined simulation model that contains both discrete and continuous state change behaviour). The size of each small time interval is calculated separately and depends on the required accuracy.

To summarise, transient behaviour is described by states and rates. State equations are direct representations and differential equations are indirect representations of variables that describe the state of the system. State equations are easy but differential equations difficult to solve and require numerical integration that involves the advancing of the simulation model time in small time intervals.

It is essential to note that simulation models that are developed with both the original simulation modelling method and the generic simulation modelling methodology do not make provision for transient behaviour. It is assumed that the changes in the state of the system occur at isolated points in time (see the behaviour of the Discrete State Change on Time B of Figure 1.6).

The reasons why this assumption is made are the following:

a) Both the original simulation modelling method and the generic simulation modelling methodology provide decision support on a strategic level (see Section 1.1). Therefore the level of resolution (see Section 1.2) that is required excludes transient behaviour.

b) The managers of plants usually strive towards the maximisation of the throughput and as a result the bandwidth of variation that occurs during changes in the state of the system is generally restricted to a small range (typically less than 10% of the total range of the state of the system). The small range of variation in the state of the system tends to negate the effect of transient behaviour.

c) Integration is basically a process that determines the area underneath a function. For example, if the rate of production of a plant over a period of time is integrated, it yields the total production of the plant over that time period. Therefore, if the state of the system that is indicated in Figure 1.6 represents the rate of production of a plant, the area underneath the function or curve represents the total production. A scrutiny of Figure 1.6 reveals that Area A is taken into account when assuming a discrete state change in the rate of production and it results in a positive fault when the total production is calculated. In a similar fashion Area B is not taken into account when assuming a discrete state change in the rate of production and it results in a negative fault when the total production is calculated. It can intuitively be deducted that if the range of variation in the rate of production is small and many changes occur in the rate of production, then the sum of the positive Area A faults is counterbalanced by the sum of the negative Area B faults.

The integrity of the assumption not to include transient behaviour is borne out by the fact that the original simulation model deviates less than 1% (0,59%) from the real-world situation for a known scenario (Albertyn, 1995:76). The fact that both the original simulation modelling method and the generic simulation modelling methodology do not make provision for transient behaviour is perceived as a possible limitation in this section but, paradoxically, it can also be perceived as a necessary and beneficial exclusion. The exclusion of transient behaviour reduces complexity and it is certainly beneficial in the attainment of the characteristics of the generic methodology that is detailed in Section 1.5.

To expand on the provision of a context for simulation models that are developed with the generic simulation modelling methodology, it might be useful to provide a very basic comparison with some other modelling methods and techniques. An LP model, for instance, is usually a static model that is strictly deterministic. The scenario that is under scrutiny in an LP model is represented as a "snapshot" of the behaviour of a system at an isolated point in time. An LP model finds the singular optimum solution to a governing set of equations and cannot investigate the behaviour of the system over a period of time or study the effect of random phenomena on the system. A detail simulation model is usually employed to investigate the dynamic behaviour of a system over a short period of time, typically in the order of milliseconds to hours. Such a simulation model is used as a decision support tool on the detail level of engineering. For example, the 3- and 6-degree-of-freedom simulation models that are used to investigate the performance of aircraft and missile systems fall within this category. A detail simulation model typically incorporates differential or difference equations and advances the simulation model in time with very small time increments, thereby achieving numerical integration of the differential or difference equations. Random phenomena are not included and a detail simulation model is therefore strictly deterministic. By comparison a simulation model that is developed with the generic methodology usually investigates the dynamic behaviour of a system over a longer period of time, typically in the order of hours to years. It is used as a decision support tool on a strategic level. Such a simulation model incorporates random phenomena and is therefore stochastic.

Summary

The simulation model classification framework that is provided in this section indicates that a simulation model of the class or type of system that is considered in this document can be classified as a dynamic, combined, stochastic simulation model. Continuous state change behaviour or transient behaviour is usually represented with state and differential equations. The generic simulation modelling methodology does not make provision for transient behaviour but this is not necessarily a limitation because it greatly simplifies the generic methodology.

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