



REAL-TIME OBSERVER MODEL

FOR A KRAFT WOOD DIGESTER

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PREFACE

Sappi Ltd initiated this project to be able to control the Kappa number value for a kraft pulp process at Tugela using a real-time estimate of its value.

The investigation required co-operation with the staff of Sappi Tugela from the digester section. Digester data were collected directly from the mill. Other studies and off-line simulations were performed in the postgraduate offices of the School of Chemical Engineering at the University of KwaZulu-Natal, Durban under the supervision of Professor Michael Mulholland.

The following courses were completed during the course of this study:

DNC4DC1 Process Dynamics and Control

DNC5RT1 Real Time Process Data Analysis

This work led to two conference presentations.

I hereby declare that this dissertation is my own work, unless stated to the contrary in the text, and that it has not been submitted for a degree to any other university or institution.



A. MOLLEREAU

Date 07/02/2005

As the candidate's supervisor, I have / have not approved this dissertation for submission

Signed: Name: Date:

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Abstract

At SAPPI-Tugela a continuous Kraft wood chip digester operates in EMCC mode (extended modified continuous cooking). Chips are initially exposed to a NaOH / Na₂S liquor at high temperature in the top section. The chips move downward in plug flow passing circumferential screens used to draw liquor for various circulations. About midway down the spent black liquor is removed and the chips enter the cooler bottom section where some further reaction and washing occurs. Liquor level and chip level are maintained close to each other near the top. Chips require 8-12 hours to pass through the digester, depending on the chip feed rate. The key parameter of interest at the digester exit is the Kappa number, which is a measure of the extent of delignification which has occurred.

Different board and paper products require different Kappa number pulp feed. (Final properties such as tensile, tear and bursting strengths will also depend on the way fibres have been modified in the digestion). The objective of this investigation is to predict the Kappa number of the product pulp in real-time, thus facilitating quicker reaction than the present dependence on laboratory analysis permits, possibly even allowing closed-loop control. The extent of delignification depends on liquor strength, temperature and exposure time, with final Kappa number also depending on the properties of the chip feed (wood type and moisture content). Compensation to maintain a steady Kappa number is made difficult by the long and varying residence time, and the fact that any changes apply to the whole profile held up in the digester.

A number of static models for Kappa number prediction have been developed by previous workers, but these do not compare well with plant measurements. The collection of data from the Sappi-Tugela reactor, and the pulp quality reports, have been used to determine an efficient model. This step required a considerable data collection exercise, and similar results to the quality reports have been obtained using a simple linear model based on this data. The problem of model error is being reduced by arrangement as a Smith Predictor, in which the model is intermittently corrected by available laboratory analyses.

At the same time, an interface was created, in order to synchronise measurement data for the chips presently leaving the reactor. In order to deal with the dead time, each parcel of chips entering the reactor is effectively tracked, and the changes in Kappa number integrated for reaction time under the varying conditions in transit. Knowing the present inventory of the reactor, this model can also be run forward in time as a predictive controller, to determine optimal control actions for maintenance of the target Kappa number.

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LIST OF SYMBOLS

Acronyms

DCS – Distributed Control System

DMT - Dynamic Modelling Technology

EMCC – Extended Modified Continuous Cooking

GUI – Graphic User Interface

IMC - Internal model control

MIMO - Multiple Inputs-Multiple Outputs

MPC – Model Predictive Control

PID - Proportion-Integral-Derivative

SISO - Single Input-Single Output

CHAPTER 1

Introduction

Pulp is said to have been invented in 105 A.D when a Chinese court official, Ts'ai Lun, mixed mulberry bark, hemp and rags with water, mashed it into pulp, pressed out the liquid, and hung the thin mat to dry in the sun. This was the beginning of a great revolution in communications.

In 1879, a German chemist, C.F. Dahl, developed the kraft (from the German word meaning "strong") pulping process.

The development of paper signalled the beginning of the modern communication era. Later innovations incorporating paper would include the development of the Gutenberg Press, which allowed for mass production of printed materials thus increasing the demand for and production of paper.

In 1954, the South African Pulp and Paper Industries Limited (SAPPI Ltd) produced its first reel of paper for kraft packaging in Tugela.

Fifty years later, the world market demands high efficiency, even in a world where electronic communication takes more and more place in our everyday life. Control is made difficult by the complex processes involved. The kraft pulping process is one of those.

The consumption of paper per head of a nation's population has been suggested to be a good indication of the degree of civilisation this nation has attained. It is clear that paper, as a means of communication, has played a great role in the development of the world we know. Paper has been used all over the world for centuries in many different ways: mail, archives, speeches. Furthermore, its robustness gives paper the ability to resist deterioration over time.

Many materials were used before the advent of paper such as papyrus, animal parchments, stones, bones, leaves and silk fabrics for example. All of them have evident limitations. Prepared from the reed of the plant with the same name, growing on the banks of the Nile,

papyrus was found in Egyptian tombs of 3500 B.C. This papyrus was a great invention as we know it served as a writing material for the great works of the Greeks and Romans until the ninth century A.D.

The skins of animals were introduced as parchments by King Eumenes of Persia about 170 B.C. Domestic animals such as calves, goats and sheep were the main source of skins. The younger the animal, the finer was the parchment.

The origin of papermaking is not exactly certain but surely happened in China. Archives gave credit to Ts'ai Lun about 105 A.D. The records indicate that he "first made paper by pulping fishing nets and rags. Later, he used the fibers of plants - any which provided sufficient elasticity in tension were used as the raw materials for paper. The raw materials were first boiled and then beaten into a mash. They were then stirred into a pulp and spread on a training frame or basket. When it had formed a thin tissue, the resultant paper was then pressed with heavy weights."

Nearly 97 % of the world's paper and board is made from wood pulp and nearly 85% of the wood pulp used is from coniferous trees. This is a logical result of the technological and sociological developments that happened in the eighteenth and nineteenth centuries in Europe and North America: it was a literary age; the mailed correspondence increased and the educated classes bought more books thus elevating the production of papers. As a result, the paper industry had to follow the laws of supply and demand and improving the paper making process was one of the solutions.

The rags used from the early days gave papers of good quality but the demand was too high and it was high time to look for other raw materials. It is fortunate that the improvements of the techniques were made in places with much coniferous forest. Wood became the other suitable material for papermaking. Conifers offer very good papermaking properties, thus allowing further improvements.

Techniques involving wood pulp were developed from 1844 when Keller and Voelter, in Germany, developed a process for mechanical wood pulp. Keller found that, instead of hammering the raw material as it was done in the early days, a better pulp was formed when the wood is held against a revolving grindstone while a stream of water wash away the particles of fibre. The quality of the pulp obtained was undeniably lower than the one made from rags. But the process was cheaper and the raw material, the wood, was in large supply. Even if enormous improvements have been made since then, the dependency of the industry has relied on wood.

Controlling quality and yield is now the next step in wood pulping. The very high demand of papers has reached a point where important financial factors are taken into account. It is essential to guarantee such levels. Process control is used to make this guarantee real.

Process control offers the potential to maintain product specification within narrower ranges. It is a challenging area as the machinery used is such that many variables may interact. Control as we know it today with sensors, computers, models, alarms and all the technological equipment that follows has not been yet fully incorporated in pulp and paper processes. As will be described in the following chapters, the Kraft process we analyse turns out to be problematic, like many industrial processes, and we can clearly imagine the difficulty without modern control.

The product targeted by this study is the blow line pulp issued from the Kraft section of a pulp and paper mill. This pulp will be used in the following part of the plant to create different papers of different qualities.

In this research project, a real-time observer model is proposed and validated. It will be part of control strategy aimed at providing stabilization to product quality.

1.1 Research objective

An observer model is proposed to analyse the production of pulp at the Sappi Tugela mill. The pulping process used is the Kraft process. This observer model is required to bridge the observation gaps and eliminate the additional delay before the laboratory results become available. When these results become available, the predictions of fundamental states and pulp properties are compared with the synchronised prediction from an historical buffer file to provide a correction.

This observer will allow the operators of the mill to get an immediate feedback on the way the digester is operating and allows necessary adjustment of some variables to get a product with better quality. A Smith predictor is used to correct the predicted values. It has turned out to be a popular dead-time compensator: when the appropriate measurement becomes available, a synchronised (old) error can be used to correct current model predictions. The next step in the study will be the implementation on-line of the model after the installation of a Distributed Control System (DCS).

The problem of Kappa number control is well-recognised in the pulp and paper industry. Many studies have attempted to predict Kappa number based on process measurements, to avoid the slow adjustment cycles resulting from reliance only on periodic laboratory analyses. It was decided to develop a dynamic model of the digestion process which will respond to the ongoing operating conditions. Online operation of the predictive model would be enabled by the installation of the new DCS. It was the perfect opportunity to implement on a manufacturing site a simple yet robust solution. Besides, the proposed model, having its own offset correction, meant that great accuracy was not mandatory.

1.2 Layout of the thesis

Chapter 2 lays the background of this study: all information needed on wood, modelling, Smith prediction and the Kraft process will be presented in this chapter.

- The wood: the nature of wood, the different types of wood, its chemistry.
- Kraft process: the process used at Sappi Tugela.
- Modelling of the Kraft digester: a comprehensive review of the work undertaken in the last decades in the field of modelling which concentrates on continuous digesters. An approach is made to mathematical modelling.
- Smith prediction and internal model control (IMC).

Chapter 3 highlights the experimental approach of the project and the work accomplished for this study. It begins with the development of the model and ends with the implementation on-line on the DCS of the model.

Chapter 4 sums up the results obtained concerning the off-line and on-line tests and the discussions following these results.

Chapter 5 concludes and closes this study. Recommendations for future research are made.

CHAPTER 2

Background

As stated in the previous chapter, this section will focus on the different backgrounds of this study.

2.1 The wood

2.1.1 Wood anatomy

Within living trees, wood is produced to perform the roles of support, conduction and storage. The support role enables the tree stem to remain erect despite the heights to which a tree grows. Because of these heights, wood must also perform the role of conduction, which is the transport of water from the ground to the upper parts of the tree. Finally, food is stored in certain parts of the wood until required by the living organism. It is important to give a definition of fibre, as this element of wood is often referred to in the thesis. According to the vocabulary of the plant anatomist, fibre is a word of restricted meaning used generally as a name for a type of cell found in the fibro vascular system of angiosperms. However, the papermaker uses the term to describe any plant cells that are the major constituent of pulp.

2.1.2 Wood chemistry

The chemical components of wood can be divided into 4 main groups: cellulose and hemicellulose, which are polysaccharides, and lignins and extractives. The first two, taken collectively, are often spoken of as holocellulose.

Cellulose determines the character of the fibre and permits its use in papermaking. It is the main component of the fibre in wood, contributing between 40 and 50% of the total dry mass of wood, depending on the species (Gullichson (1999)). It consists of linear beta-D-glucopyranose polymers with a degree of polymerisation between 10000 and 15000 before pulping.

For practical reasons, cellulose has been classified according to its solubility in an alkali solution:

α -cellulose: not dissolving in strong caustic solution

β -cellulose: precipitating when acid added

γ -cellulose: remaining in solution

The chemical structure of cellulose is shown in Figure 2-1.

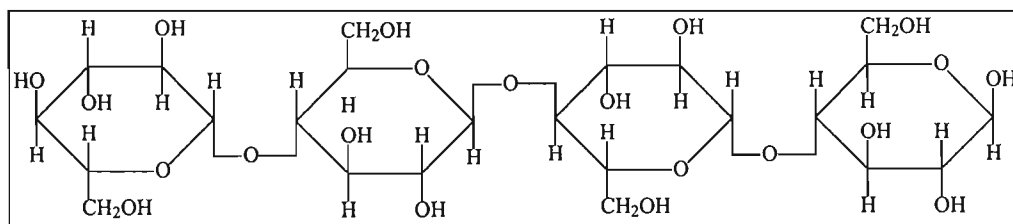


Figure 2- 1 : Chemical structure of a cellulose molecule (Smook , 2002)

The polymeric linkages are such that the chains form in an extended manner. Thus, the molecules fit snugly together, giving birth to powerful associative forces that are responsible for the great strength of cellulosic materials.

Hemicellulose, also called polyoses or γ -cellulose is found in close association with cellulose. However, they differ in that the molecular chain is shorter and has a more branched chain structure. Furthermore, hemicellulose is more soluble than cellulose.

Hemicellulose consists of different substances: it includes xylan, glucuronoxylan, arabinoxylan, glucomannan, and xyloglucan (see Fig.2-3). The function of hemicellulose is poorly understood: It's too small for structural support. It may have a water transport function. The degree of polymerisation stands between 150 and 200. Nevertheless, it has a positive impact on the bonding strength of fibres. Indeed, the chains form a 'ground' - they bind with pectin to cellulose to form a network of cross-linked fibres. Hemicellulose is more easily degraded and dissolved than cellulose, so the percentage is always less in the pulp than in the original wood. The third component is the lignin. It's an aromatic polymer with a complex structure. It represents 17 to 33% of the dry wood mass. All lignin is based on 3 units: p-coumaryl alcohol, coniferyl alcohol and sinapyl alcohol (chemical structure shown in Figure 2-2).

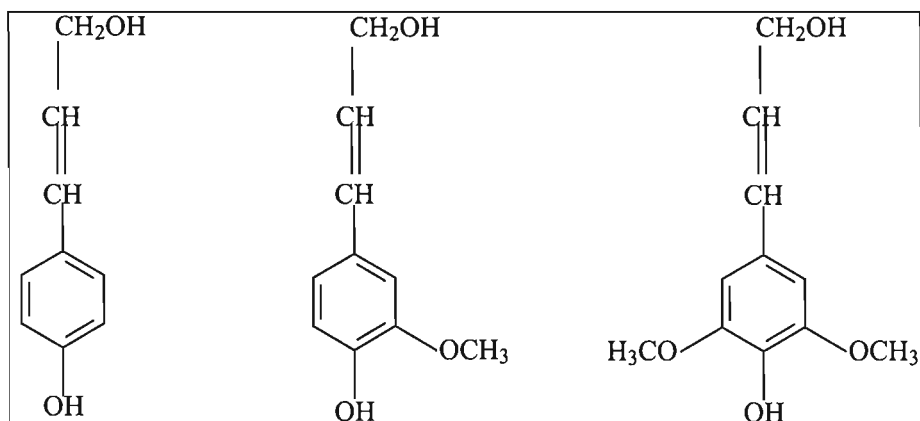


Figure 2- 2: The building units of lignin: p-coumaryl alcohol, conyferyl alcohol, sinapyl alcohol (Kocurek and Stevens, 1983)

These units are linked together in many different ways, mainly by oxygen (ether) bridges connecting the alpha or beta carbons of the side chain of one unit with the phenyl ring of the other.

<u>Hemicellulose type</u>	<u>Simplified structure</u>		
Galactoglucomannan	$ \begin{array}{cccccccc} G & - & M & - & M & - & M & - & G & - & M & - & M & - & M & \cdots \\ & & & & & & & & & & & & & & \\ & & \text{GAL} & & \text{Ac} & & \text{Ac} & & & & & & & & \text{GAL} \end{array} $		
Glucomannan	$G - M - M - G - M - \cdots$		
Arabinoglucuronoxylan	$ \begin{array}{ccccccccc} X & - & X & - & X & - & X & - & X & - & X_5 \\ & & & & & & & & & & \\ & & \text{Ga} & & & & \text{a} & & & & \end{array} $		
Glucuronoxylan	$ \begin{array}{ccccccccc} X & - & X & - & X & - & X & - & X & - & \cdots \\ & & & & & & & & & & \\ & & \text{Ac} & & & & \text{Ga} & & & & \end{array} $		
Arabinogalactan	$ \begin{array}{ccccccc} \text{GAL} & - & \text{GAL} & - & \text{GAL} \\ & & & & \\ \text{GAL} & & \text{R} & & \text{A} \\ & & \vdots & & \\ \text{GAL} & & & & \text{A} \end{array} $		
<u>Abbreviations:</u>			
G	glucose	X	xylose
GAL	galactose	A	arabinose
M	mannose		
Ac	acetyl group (CH ₃ OH)		
Ga	4-O-methyl-gluronic acid		
R	usually galactose		

Figure 2- 3: The types and simplified structures of the major hemicelluloses in wood (Ingruber, Kocurek and Wong, 1985)

The units form complex macro-molecules which strengthen the wood structure and can be seen as the “glue” that keeps the polysaccharides together.

The extractives represent generally less than 5% of the wood that can be extracted using organic solvents. There are alkanes, fatty alcohols and acid glycerol esters waxes, resin acid terpenes and phenolic components. Most of these substances are soluble in water. The turpentine and tall oil are extracted during the pulping process. The extractives cause pitch deposits on the processing equipment.

2.1.3 Cell wall structure

Cellulose molecules are aggregated into threadlike structures approximately 3.5 nm in diameter, containing both crystalline and amorphous regions. These are encased in a shell of hemicellulose molecules and are called microfibrils. In the fibre wall, these microfibrils occur in small bundles or “macrofibrils”. These form thin sheets or ‘lamellae’, which gives the wall a layered texture. A diagrammatic sketch of a typical fibre is shown in Figure 2-4. A cementing layer, the middle lamella, holds the individual fibres in the structure together and is composed mainly of lignin. The middle lamella is important in any pulping process since it has to be broken or removed to separate individual cells to produce single fibres.

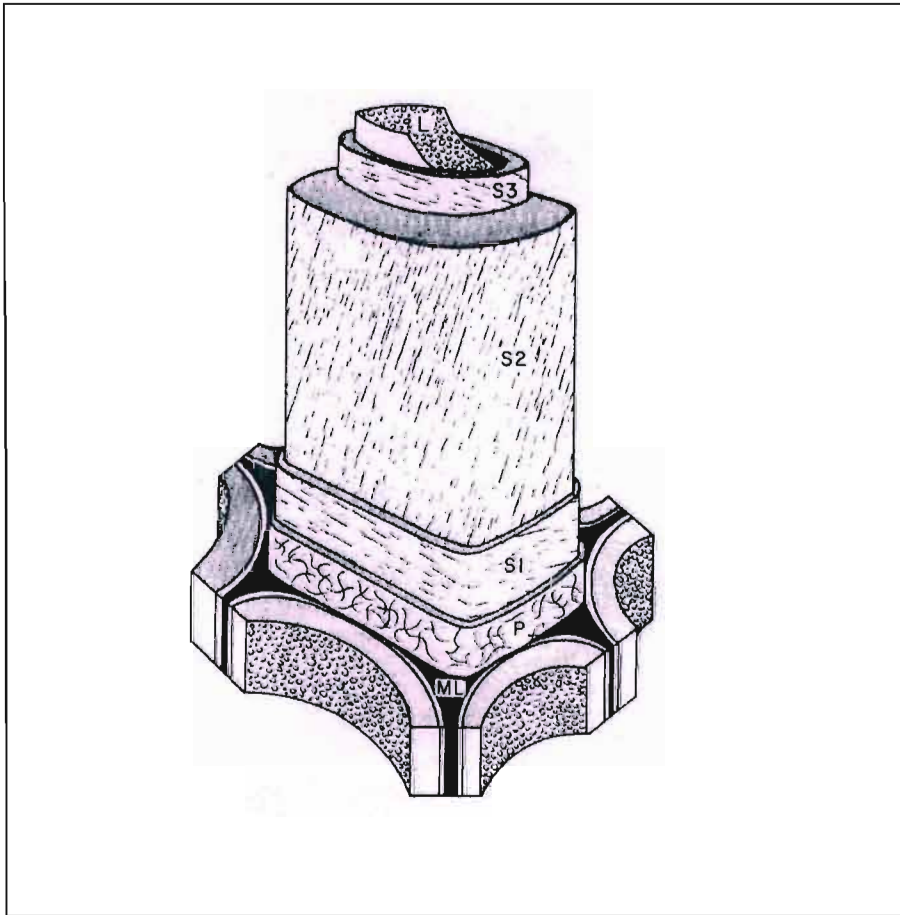


Figure 2- 4 : Layers of softwood tracheids (Smook, 1994)

ML: middle lamellae – bond between fibres, mostly lignin

P: primary wall – a thin, relatively impermeable covering about 0.05 μm thick

S: secondary wall – makes up bulk of cellwall; forms three distinct layers characterized by different fibril alignments:

S1 is the outer layer of the secondary wall (0.1 to 0.2 μm thick)

S2 forms the main body of the fibre and is from 2 to 10 μm thick

S3 is the inner layer of the secondary wall (about 0.1 μm thick)

T: tertiary wall – same as S3

L: lumen – the central canal of fibre (void)

Fibres in all plants grow from the outside inwards. When growth of an individual cell begins, the primary cell wall is formed and is initially filled with liquid. It is about 0.1 μm thick and has a netlike structure of microfibrils in an interwoven pattern. The microfibrils are orientated at an angle of about

85° with the cell axis. The primary wall is estimated to consist of only 10% cellulose embedded in an amorphous plastic matrix of hemicellulose, extractives and lignin.

The multi-layered secondary wall is formed after further growth. The outer layer of the secondary layer, called the S₁-layer, is about 0.1 to 0.2 µm thick with a microfibril angle between 50 to 70°. The S₁-layer is rich in lignin and closely resembles the primary wall to which it is closely attached, therefore also is known as the transition layer. The central secondary wall, the S₂-layer, is attached much less firmly to the S₁-layer. A continuous envelope of hemicellulose between these layers is thought to cause this lesser cohesion. The S₂-layer contains more cellulose and less lignin than the S₁-layer, whilst the microfibril angle is between 10 and 30°. It forms the bulk of the fibre and is about 2 to 6 µm thick.

The tertiary wall is the innermost component of the cell wall and surrounds the central canal called the lumen. The tertiary wall is very thin, about 0.1 µm, and is rich in hemicellulose.

2.1.4 Wood classification

Trees are classified into two major groups, namely softwoods and hardwoods. The botanical basis for classification is whether or not the tree seed is naked as in softwoods or covered as in hardwoods. The major difference with regard to wood anatomy is the presence of vessels in hardwoods. Vessels are structures composed of cells created exclusively for the conduction of water. Softwoods lack vessels but have cells termed longitudinal tracheids which perform a dual role of conduction and support. In general, softwood fibres are more than twice as long as hardwood fibres. Usually, softwoods are conifers, from the gymnosperms family whereas hardwoods are broad-leafed trees, from the angiosperms family.

2.1.4.1 Softwood anatomy

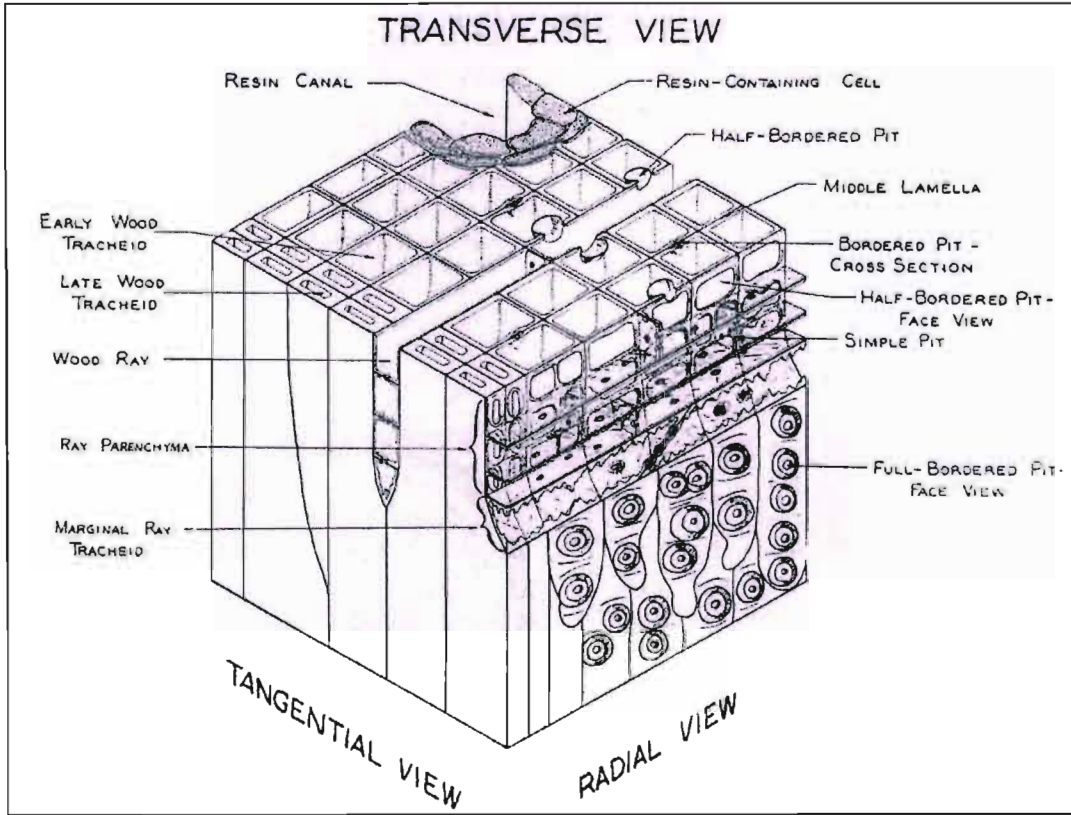


Figure 2- 5: Composite wood block illustrating the structural features of a softwood (Hyland)(Smook, 1994)

The anatomy of softwoods is a lot less complex than that of hardwoods. The two main cell types which constitute softwoods are tracheids and parenchyma. Tracheids are long, tapering cells which are orientated in the longitudinal direction, i.e. parallel to the vertical axis of the tree. Depending on species, most softwoods have tracheids ranging from 2.5 mm to 7 mm in length. The tracheids are a lot longer than the parenchyma cells, and constitute 90% or more of the volume of wood in the tree. The tracheids perform the roles of water conduction and support within a tree.

Parenchyma are responsible for storing various extractives, including starch, polyphenols, oils, fats as well as inorganics. The cells are orientated in the transverse direction, at right angles to the vertical tree axis, and are very short, chunky, thin-walled fibres. Ray tracheids, which are similar in size to parenchyma, and longitudinal parenchyma cells are found in small quantities in some softwood species.

2.1.4.2 Hardwood anatomy

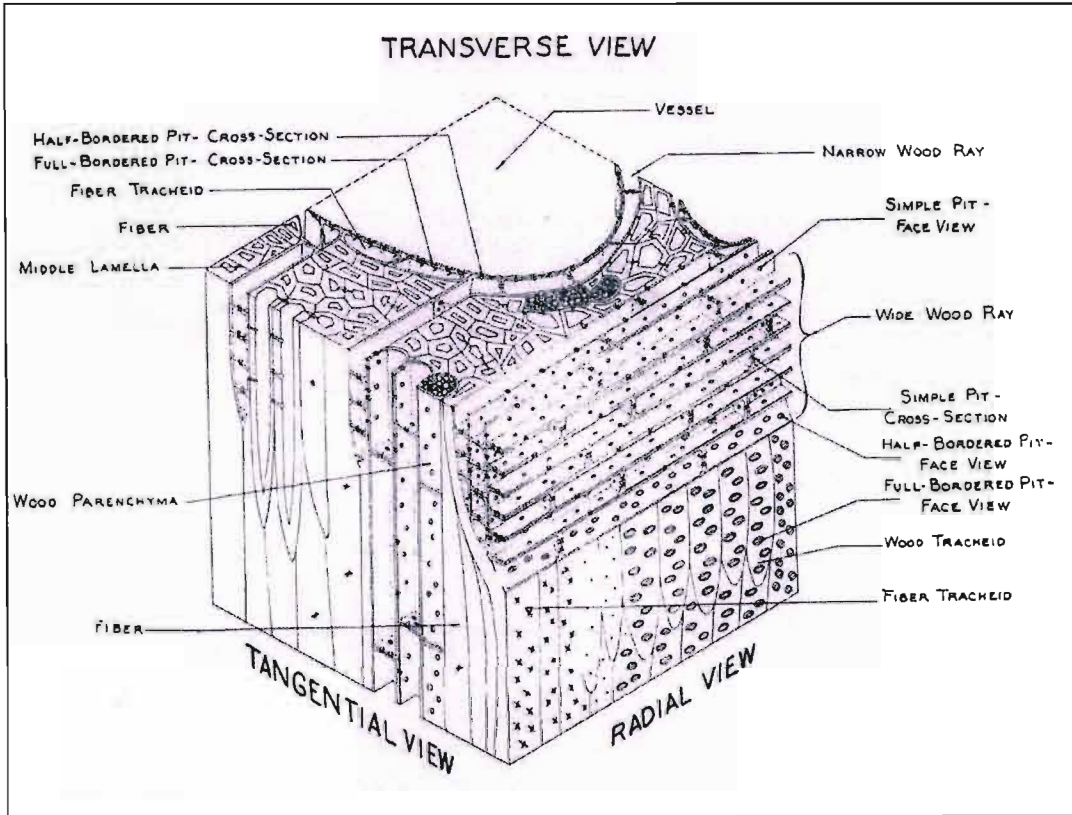


Figure 2- 6 : Composite wood block illustrating the structural features of a hardwood (Hyland)(Smook, 1994)

Hardwoods have a more complex anatomy since more than two kinds of cells are present. Specific characteristics of the hardwoods are a lack of radial alignment of cells, variable size and composition of cells, abundance of rays and the presence of pores or vessel elements. The four major cell types are fibres, vessel elements, tracheids and parenchyma cells. Each species is distinguished through the quantities of the different cells listed.

Vessels, in a typical hardwood sample, are often large enough in diameter to be seen easily with the naked eye.

Hardwood tracheids occur in small amounts in some species. These are small, longitudinal conducting cells which act as transition elements between major cell types.

2.1.4.3 Softwoods vs. hardwoods

The difference between softwoods and hardwood mainly lies in the length of the fibres. Softwood fibres are more than twice as long as hardwood fibres at the same age.

A relationship exists between wood density and a number of pulping measurements. Thus, the yield of pulp per unit volume of wood is usually directly related to density. A high wood density generally indicates a slower beating response for the pulp, lower tensile, burst and fold strengths, greater bulk and higher tear strength. Hardwoods tend to have a higher density than softwoods. Generally, hardwoods contain less lignin as compared to softwoods, but a greater percentage of extractives.

2.2 The Kraft Process

Pulping consists of reducing wood, or other fibrous raw material, to a fibrous mass. Technically, it is the way used to break the bonds within the wood structure. This task can be done in numerous ways: mechanically, thermally, chemically or by combination of these treatments. Commercial processes are then classified into mechanical, chemical or hybrid processes.

Mechanical pulping is the first process invented. A major method is the groundwood process, where a block of wood is pressed lengthwise against a revolving stone, wet and rough. Fibres are extracted from the wood and washed from the surface of the stone with water. Fibres and fragments of fibres are then screened and thickened, by removal of water, to form a pulp stock suitable for papermaking. There are of course more advanced processes, this being just a short description of mechanical pulping. These processes tend to convert up to 95% of the dry weight of the wood into pulp. But they need a huge quantity of energy to do so. Softwoods are generally used in mechanical pulping as they are more resistant than hardwoods.

Chemical pulping uses different combinations of chemicals, and also physical actions, to perform the process. The wood chips are cooked in an aqueous solution at elevated temperature and pressure. The goal here is to extract the lignin from the cellulose components and to try to leave the fibres intact. The process is quite successful in that most of the lignin is removed. However, the yield of pulp is low relative to mechanical pulping methods-between 40% and 50%. The two principal chemical processes are the sulfite process and the Kraft process. The latter is the one this study is about and will benefit from a longer description in the following chapter.

The sulfite process utilises a mixture of sulphurous acid and bisulfite ion to attack and solubilise the lignin. Sulfites combine with lignin to create salts of lignosulfonic acid. This acid is soluble in the cooking liquor. Sulfite pulping can be processed through a wide range of pH.

“Acid sulfite” characterises pulping with an excess of free sulphurous acid (pH 1-2) while “bisulfite” cooks are carried out under less acidic conditions (pH 3-5).

The sulfite process works well with softwoods and hardwoods but resinous softwoods and tannin-containing hardwoods cause some problems. Furthermore, sulfite pulps are light in color but the paper sheets are weaker than the equivalent ones in the Kraft process. These two elements, sensitivity to woods and weakness, together with a greater difficulty in chemicals recovery, are the reasons why sulfite processes are less and less used today compared to the Kraft process.

Generally, the principal factors for making paper are:

- suitability of fibre
- constancy of supply
- cost of collection, transportation and preparation
- tendency to deteriorate in storage

In 1853, Watt and Burgess patented a process concerning the cooking of wood with sodium hydroxide under pressure. Free fibres were obtained from hardwoods with enough alkali. With softwoods, the process was not advanced enough and the pulp produced was weak and brittle. Like some of the greatest discoveries, the solution came accidentally. In 1879, a German chemist, named C. F. Dahl tried to add sodium sulfate instead of carbonate as make-up chemical in the recovery process. Indeed, sodium carbonate is quite expensive. The soda pulping became sulfate pulping, and eventually the high strength of that pulp gave the name Kraft process; indeed, “Kraft” means strong in German. This way of operating increases delignification and produces a much stronger pulp. He obtained a patent in 1884.

There were two problems though: the pulp was dark-coloured and the bleaching was difficult. Hence, this pulp was not dedicated to white and printing papers. Development of the packaging papers made this brown pulp a better choice. A new bleaching method in the 1930’s, with the Tomlinson recovery furnace, along with chlorine dioxide bleaching 20 years later, developed by Howard Rapson, corrected this shortcoming concerning the use of the Kraft process for white papers.

In the 1950’s, the development of the bleached hardwood Kraft process made it possible for the process to enter the market of fine papers. This was directly competing in the sulfite process domain.

Today, the Kraft process covers entirely the markets for wood pulp and paper.

2.2.1 Nomenclature

The cooking liquor containing the two active chemicals, sodium hydroxide (NaOH) and sodium sulfide (Na₂S), is called *white liquor*. The residual *black liquor* with the reaction products of delignification is concentrated and burned in the recovery furnace to yield an inorganic smelt of sodium carbonate (Na₂CO₃) and sodium sulfide. The smelt is dissolved to form *green liquor*, which is reacted with quick lime (CaO) to convert Na₂CO₃ into NaOH and regenerate the original white liquor (See Figure 2-7).

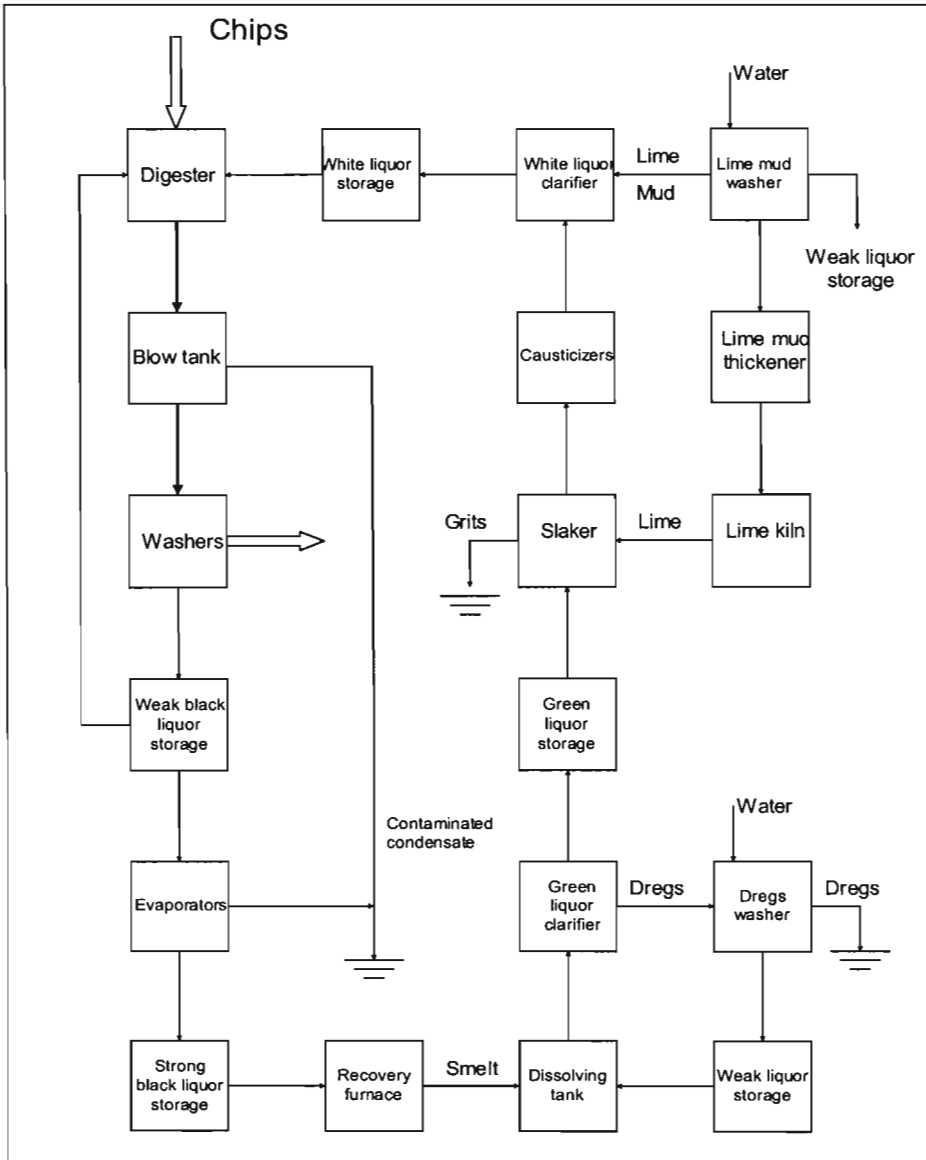
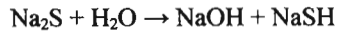


Figure 2-7: Outline of Kraft process (Smook, 1992)

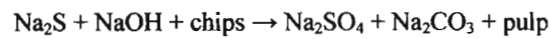
Active alkali or effective alkali supplies the better measurement of active chemical concentration for the Kraft process. Even if NaOH and Na₂S are both implied in the cooking reactions, it can be said that NaOH has the leading role, since Na₂S hydrolyzes in solution



The average composition of the white liquor is:

- NaOH 100 g/L
- Na₂S/NaSH 30 g/L
- Na₂CO₃ 20 g/L

The complete reaction could be summarized as follows:



2.2.2 Description

The Kraft process, like the sulphite process, is a method of separating the lignin from the cellulose, leaving the latter, with associated carbohydrates, as pulp (refer to Figure 2-11 for a picture of a Kraft digester). The schematic in Figure 2-9 gives a good idea of the sequential and recycle aspects of the Kraft process. The Kraft process can be either batch or continuous.



Figure 2- 8: Some chips from Sappi Tugela mill

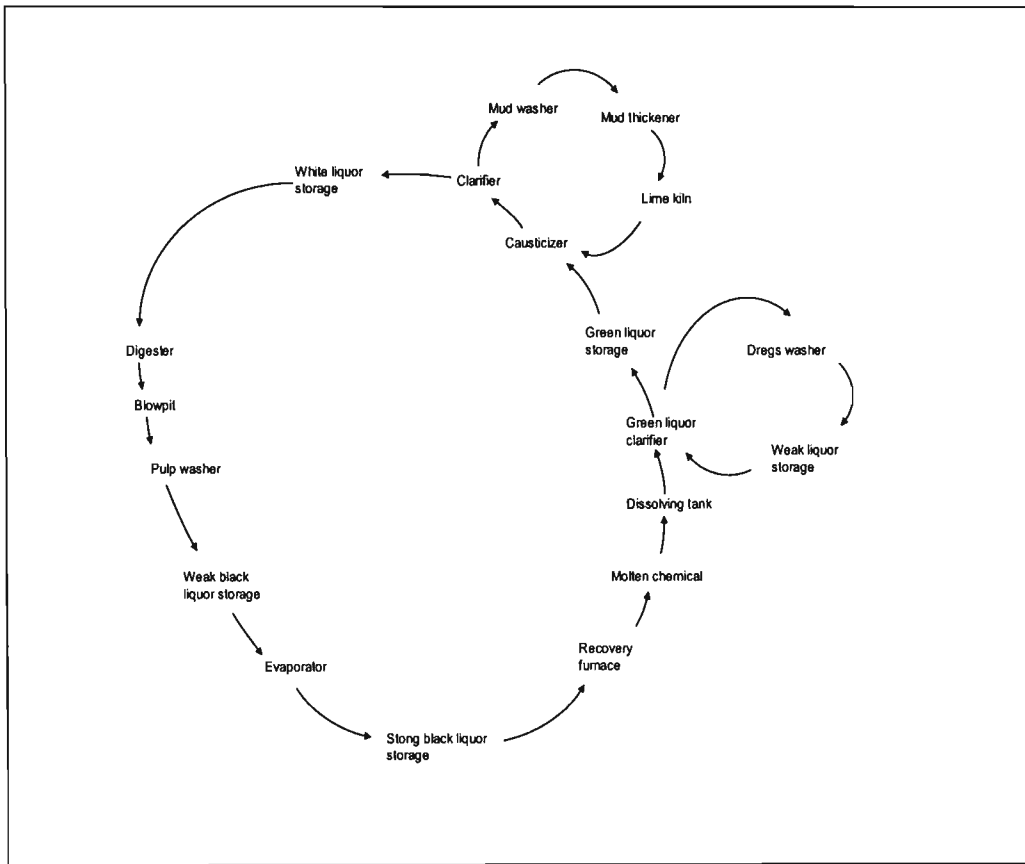


Figure 2- 9: Diagram showing cyclic nature of the Kraft recovery process (Leske, 2002)

For the batch cooking, cooking liquor covers the chips in the digester vessel (See some chips in Figure 2-8). Steam jets are used to obtain a good packing and thus a low liquor to wood ratio. Then, the system is heated, usually by a forced circulation of the cooking liquor through heat exchangers. Gases are generally relieved through a pressure control valve at the top of the digester. After 60 to 90 minutes, the maximum temperature is reached and the cooking liquor impregnates the chips. Then, the cook is maintained around 170°C for up to 2 hours to complete the cooking reactions. Once the digestion is complete, the contents are discharged into a blow tank where the softened chips are disintegrated into fibres.

For the continuous cooking, chips are first carried through an impregnation vessel, known also as the steam vessel (see Figure 2-10) where the air is removed from the pores. Tugela mill is using a mixture of both hardwoods and softwoods with an unknown distribution. The steam is provided by a dedicated low pressure steam stream. The flow is manipulated to control the pressure within the impregnation

vessel. The chips and liquor enter the digester (zone I, Figure 2-12) along with fresh liquor at a temperature around 120°C. A dedicated high pressure steam stream maintains the pressure and thus the temperature at the top of the digester. The pressure needs to follow a certain set point according to the chip supply flow. This pressure is often above 1700 kPa. This ensures a positive chemical penetration. Another important point is the fact that the digester is filled at all times with cooking liquor leaving no gas space. As the chip mass moves down through the digester, the mixture is heated to the cooking temperature, either by forced circulation of liquor through a heat exchanger or steam injection, and maintained at this temperature for 60 to 90 minutes. The cooking time can be reduced by increasing the sulphide content of the white liquor.



Figure 2- 10: The steam vessel

The chips and liquor next enter the first cooking zone (zone II, Figure 2-12). The temperature is raised to about 150°C by two cooking circulation systems. High pressure steam is used as a heating medium. Temperature controllers for the liquor set up the precise desired temperatures.

After the first cooking zone, the chips and liquor penetrate into the second cooking zone (zone III, Figure 2-12). Most of the delignification process happens in this zone as a certain temperature is needed, usually above 140°C. The reaction rates in delignification are dependent on alkali dosage, temperature and time. The H-factor takes into account time and temperature and is generally the

parameter used to predict the Kappa number. A H-factor of 870 corresponds traditionally to a Kappa number of 80.

Finally, the chips reach the washing zone (zone IV, Figure 2-12). This zone is a counter-current zone where wash liquor is injected to slow down the delignification reaction. The remaining liquor chemicals are extracted from the chips here. Thus, the fibre characteristics are preserved as the chemical content is low. The pulp is then transferred out from the digester.

Fresh white liquor is introduced in the impregnation zone (zone I, Figure 2-12), in the second cooking zone (zone III, Figure 2-12). Fresh white liquor is also introduced in the recirculation flows (zones II to zone I, Figure 2-12) and in the washing zone (zone IV, figure 2-12). Every flow is being controlled to avoid any overflow. This is especially true when changing the production rate.

The alkali dosage is 13.0 % Na₂O on dry wood (mass/mass). The total volume of the Tugela digester is 1390 m³. In this case, the entire digester is a cooking zone. The way this digester is designed allows a greater production rate but also gives more variation in the Kappa number values when disturbances occur than a traditional digester where only a part of it is dedicated to the cooking.

The hot spent liquor is extracted into a low-pressure tank where flash steam is generated for use in the impregnation vessel. The pulp is generally lowered below 100°C with cool liquor to prevent any mechanical damage to the fibres. The cooked pulp is then separated from the residual liquor in a carefully controlled process known as brown stock washing. The most common method employs a series of counter-current vacuum drum washers to provide displacement of the liquor with minimum dilution. Some continuous digesters incorporate a diffusion washing step in conjunction with spent liquor extraction and pulp cooling. Following washing, the pulp is screened and cleaned. These operations are both important to the production of high-quality Kraft pulp.

As the environmental issues became more and more important, and as the pulp and paper industry is a great consumer of chemicals, the reduction of chlorine and chlorine dioxide consumption in the bleach plant became an important issue. To reduce the chemical consumption it's necessary to lower the lignin content (i.e. Kappa number) of the bleach plant feed stock.

One method aimed at producing a low Kappa pulp from the digester while maintaining pulp strength is to use extended modified continuous cooking (EMCC). The Tugela mill is using such a digester. The EMCC process divides the cook zone into co-current and counter-current regions and distributes the white liquor charge to a number of additional points. The results are a more uniform alkali profile throughout the digester. This cooking also allows lower Kappa numbers to be achieved while

maintaining a high viscosity (high fibre length). From an environmental viewpoint, the EMCC cooking results in significant reductions of bleaching chemicals (Martin, 2000).

The digestion is really at the beginning of the paper cycle. Different pulps can be manufactured given the sources: waste paper, after being de-inked, is often used to produce linerboard or fluting. Untreated wood pulp has a brown or brownish colour and has to be bleached before it can be used to make white papers. This is done in a bleaching plant.

The bleached pulp is then refined to give it the exact properties wanted. At the refiner, the pulp passes through a system of rotating and stationary blades which fibrillate the fibres to enhance the way they mesh together and cause the bonding properties of the fibres to be increased. From different pulp grades (pulp produced from softwoods or hardwoods), a mix is produced and then introduced into the paper machine. Some chemicals can be added to get the wanted quality: opacity, smoothness, liquid penetration. Off-line coating and calendaring finish the paper-making process.

Off-line coating consists of optimizing the printing characteristics of the paper. It may be applied on the base paper.

Calendering is another optimization process that can be applied off-line or on-line. It develops the smoothness and gloss on the surface of the paper.

Then, the end-product is cut to the size specified by the customer and packed in reams, reels or simply sheets.

Sappi runs four different paper machines (PM) at Tugela Mill. PM1 produces high-yield fluting. The PM2 produces kraft linerboard and premium high performance containerboard. The PM3 is solely manufacturing machine glazed paper. Machine glazed paper is commonly used for printing bags, wrappers and posters. Finally, PM4 deals with extensible sack kraft paper.

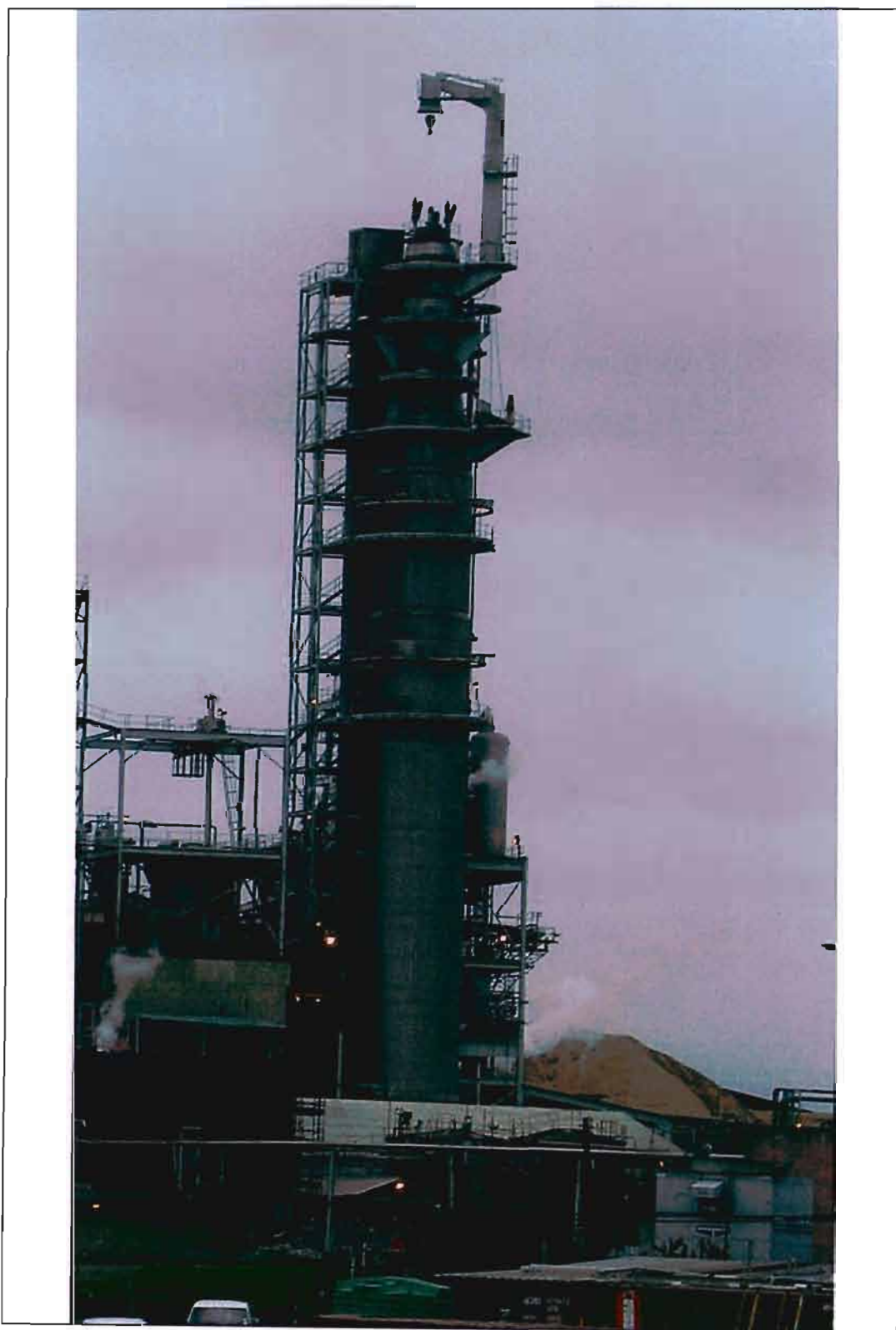


Figure 2- 11. The Sappi Tugela Kraft digester

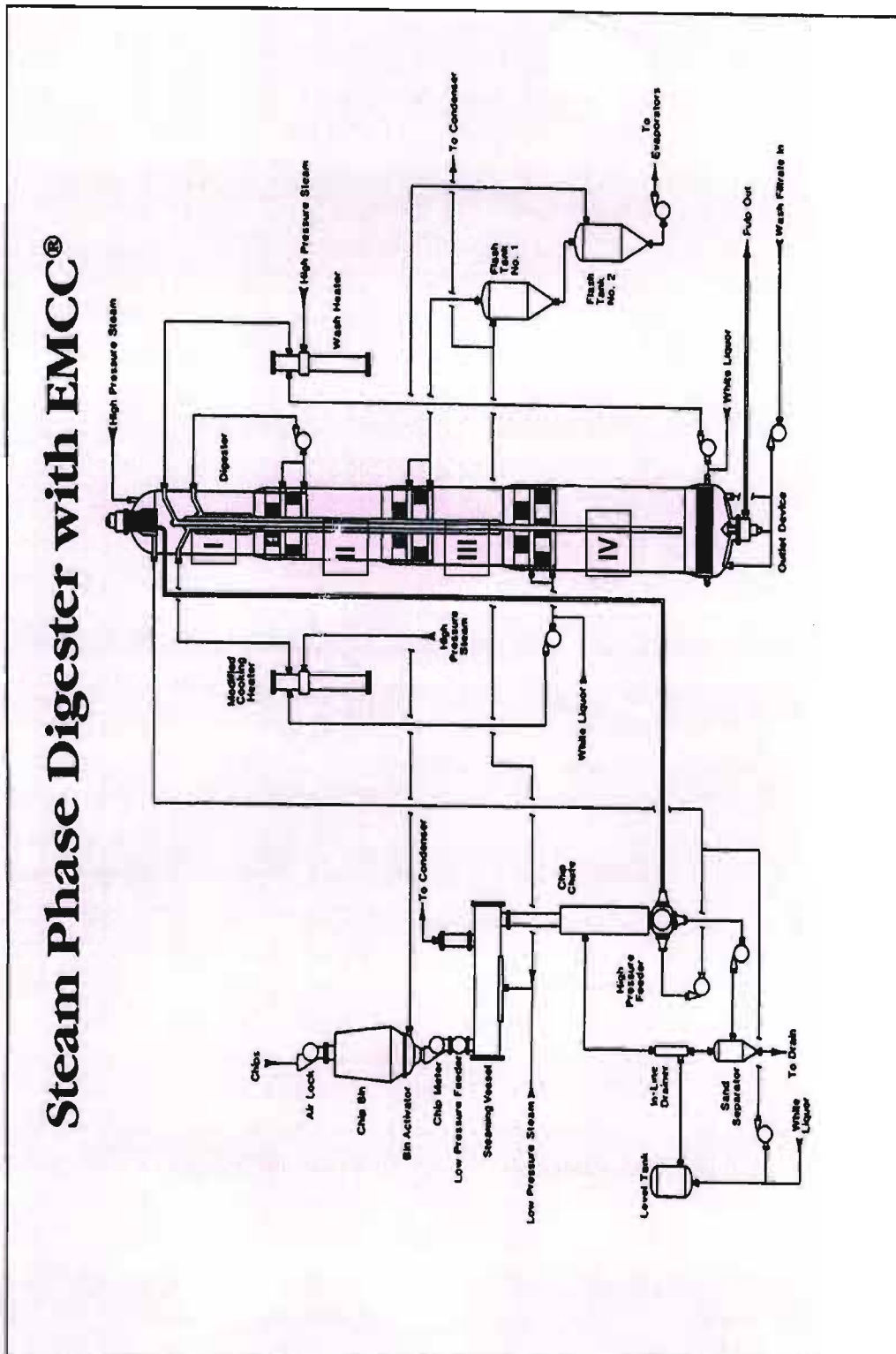


Figure 2- 12 : Schematic of a Kraft digestion process with EMCC (Sappi Tugela technical documentation)

2.2.3 Chemical recovery

The black liquor, mentioned as a constituent of the cooking liquor, is the dilute liquor resulting from the middle washings of the pulp in the diffusers. It is then treated in a series of steps to recover the cooking chemicals and regenerate the cooking liquor. The concentrated liquor from earlier washings is sent to the chemical recovery plant and the very dilute liquor from the end washings is sent to the drain. The concentration of black liquor is controlled by analysis.

This process is completely integrated in the Kraft mill operation.

The weak black liquor, composed of 15% of solids, arising from the brown stock washers, is processed through a succession of actions:

- 1- concentration through a series of evaporation and chemical additions steps into “heavy black liquor (70-75% of solids)
- 2- incineration of heavy black liquor in the recovery furnace to form inorganic smelt
- 3- dissolving of furnace smelt in water to form green liquor
- 4- causticizing of green liquor with reburned lime to form white liquor for the next cooking cycle

An important function of the recovery furnace is to chemically reduce the oxidized sulphur compounds contained in the burning solids to sulfide. This aspect of furnace operation is monitored with measurements of reduction efficiency.

Control of green liquor strength is essential for smooth operation within the liquor cycle. The target level is a compromise between two factors. A higher concentration increases the inventory of soda chemicals, which help to level out the operation and provide surge capacity against interruptions. Nevertheless, a lower concentration improves causticizing efficiency, ensuring that a lower “dead load” of non-reactive Na_2CO_3 will be carried around the cycle.

2.2.4 Chemistry of Kraft pulping

The reactions occurring in the digester are complex and not entirely understood. The main reaction is believed to have the kinetic characteristics of a unimolecular reaction, but influenced by the rate of diffusion of the lignin. Technically, the swollen lignin in the wood chips is chemically split into fragments by the hydroxyl (OH) and hydrosulfide (SH) ions present in the pulping liquor. The lignin fragments are then dissolved as phenolate hemicelluloses and some cellulose, are also chemically attacked and dissolved to some extent. During a typical cook, approximately 80% of the lignin, 50% of the hemicelluloses and 10% of the cellulose is dissolved.

Given the right conditions, the lignin fragments are able to take part in condensation reactions either with themselves or undissolved lignin and possibly with carbohydrates. The condensed lignin is more difficult to remove from the fibres. The hydrosulfide ion is believed to reduce condensation reactions by blocking reactive groups.

The two driving forces for Kraft pulping reactions are alkali concentration (either effective or active alkali) and temperature. Within the normal cooking temperature range (155-175 °C), the delignification rate more than doubles for every 10°C increase.

By arbitrarily fixing a relative reaction rate of 1 for 100°C, a method has been developed for expressing the cooking time and the temperature as one single variable. When the relative reaction rate is plotted against the cooking time in hours, the area under the curve is defined as the H-factor. The concept of the H-factor has been widely applied in cooking control, but is especially useful when the temperature varies during the cooking period.

The delignification reaction is assumed to be first-order, parameterised with a single rate-constant K. Thus the H-factor can be calculated as:

$$H = \int_0^t \frac{K_{T(t)}}{K_{373}} dt = \int_0^t e^{\left(43.181 - \frac{16113}{T(t)}\right)} dt \quad (2.1)$$

The division delimited in red is a relative rate constant for the delignification. Delignification during Kraft processing proceeds in three distinct phases as shown in Figure 2-13.

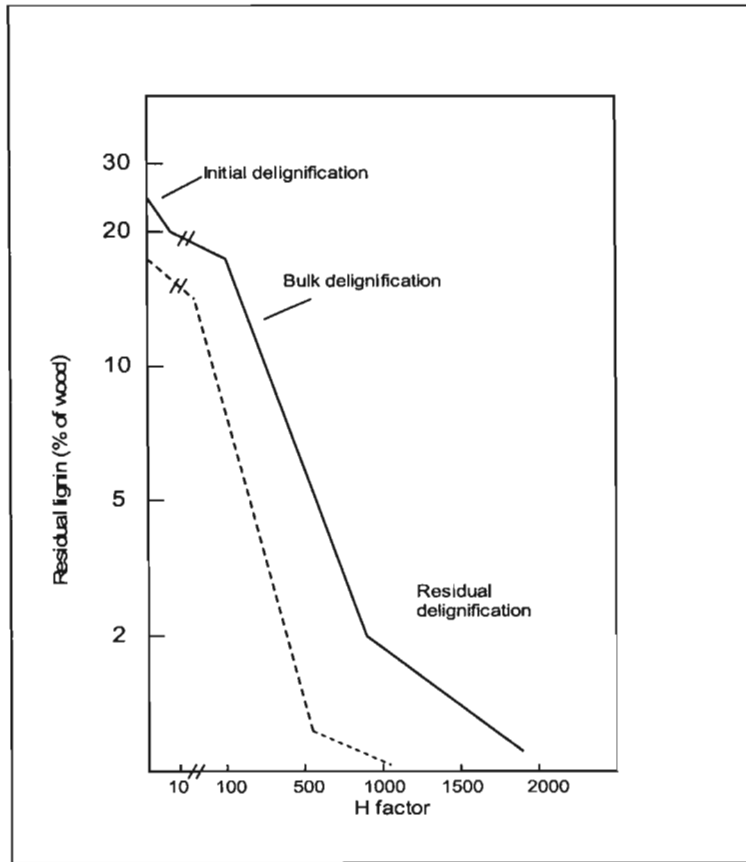


Figure 2-13. Removal of lignin during Kraft pulping of pine (—) and birch (---) as a function of H factor (Kleppe, 1970)

The initial and very rapid lignin removal is characterized as an extraction process. Removal of the bulk of the lignin follows as a first order reaction. Kraft cooks are typically completed at a lignin content of 4-5% for softwoods and about 3% for hardwoods, well within the bulk delignification phase. If cooks were allowed to proceed further, residual delignification would occur at a much lower rate.

The following list gathers the basic variables affecting the Kraft process:

- Wood chips:
 - species
 - general chip quality
 - moisture
- Cooking liquor
 - sulfidity
- Cooking control
 - liquid to wood ratio
 - temperature cycle
 - H-factor
- Control parameters
 - degree of delignification

As with most chemical pulping methods, sufficient time is needed at a lower temperature to achieve a good liquor penetration into the chips before the main cooking reactions occur. Insufficient impregnation lowers the degree of cooking and increases the level of screen rejects. Since air in the chips can interfere with penetration, it has been found useful in continuous system to presteam the chips to expel the air.

2.2.5 Effect of chip size

Reduction in chip thickness allows faster pulping rates and reduces the amount of screen rejects. Generally, smaller-length wood fragments like pin chips, fines and sawdust produce lower yield, weaker pulps and consume greater amounts of alkali. A high percentage of fine material in the chip furnish will cause poor liquor circulation. It's advised to cook this material separately.

The particle size and its distribution of chips used for Kraft pulping are known to play an important role in achieving a uniform cooking result. Poor uniformity results in excessive loading of pulp and rejects handling equipment and excessive chemical usage in both cooking and bleaching. The quality of chips entering the process must be properly watched.

2.2.6 Effect of liquor sulfidity

Compared to soda pulping, Kraft processing of softwoods is faster and provides a stronger pulp with a higher yield.

2.2.7 Effect of alkali charge

The normal alkali requirement for Kraft pulping is about 12 to 14% m/m effective alkali on dry softwoods with 8 to 10% m/m for hardwoods. It is recommended to provide sufficient chemical to carry out the reactions to completion. Furthermore, a slight excess of chemicals is used to maintain a driving force and prevent redeposition of lignin onto the fibres.

Usually, we use the minimum practicable alkali charge and vary the cooking temperature to achieve the desired reaction rate. However, a higher alkali charge also causes a slight reduction in hemicellulose retention at a given Kappa number and changes the composition of the retained hemicelluloses.

2.2.8 Effect of maximum temperature

The choice of top temperature affects the cooking result. It has to be noted though that above 180°C, losses in both strength and yield become significant due to attack on the cellulose. The chain length is shortened and the viscosity of the resultant pulp is lowered.

2.2.9 Effect of liquor to wood ratio

To ensure a good impregnation, sufficient volume of liquor is needed so that all chip surfaces are wetted. Ratios usually range between 3 and 5. The effect of greater dilution is to decrease the concentration of active chemical and then, to reduce the reaction rate.

2.2.10 Comparison between the two processes

The sulphite process is less and less used for two reasons (Hardman and Cole (1960)).

- 1- Condensation of the lignin during cooking leads to a large wastage of wood.
- 2- The large quantities of resin in the wood appear in the resultant pulp, thus, the produced pulp is one presenting high pitch-forming tendencies, causing problems in the papermaking chain.

The Kraft process has an advantage concerning the choice of woods, as both softwoods and hardwoods are compatible with this process. All the chemicals used for the making of pulping liquor are recovered. And unlike the sulphite process, there is no effluent problem.

Nevertheless, the smell is unpleasant. As a consequence, the mills that employ the Kraft process are not located near towns of any size.

2.2.11 Comparison between sulphite and Kraft pulps

→ Sulphite process

The hemicelluloses degraded during the cook are those towards the inside of the fibre. The remaining celluloses are reasonably easily accessible. The beating of pulp is fairly rapid in the initial stages compared with a Kraft process. A beater beats and crushes raw material, bruising and driving water inside the fibre and creating thread-like hairs called fibrils which are still attached to the fibre. A good fibrillation results in a stronger paper

→ Kraft process

The Kraft process allows high tear characteristic. There is a fast increase of burst factor as compared with the slow breaking length changes.

It is important to consider the Kraft process as a whole process including bleaching. Indeed, considerable quantities of resistant and highly coloured lignin are left in the pulp. Hence, the bleaching of Kraft is a continuation of the Kraft process.

2.2.12 Moisture content

The moisture content is expressed in per cent of the weight of oven dry wood. The usual method consists of weighing a sample and drying it in an oven at a temperature of 100 to 105°C until the sample ceases to lose weight. The weight lost is considered to be the weight of water contained originally in the sample and this is expressed in per cent of the final weight of the wood in oven dry condition. This way of expressing the moisture content simplifies computations.

2.2.13 Variation in strength

Strength and other physical properties of wood vary a great deal when the amount of moisture present in the wood is less than 30%. When the amount of moisture is above 30% (based on oven-dry weight), the strength remains practically the same, no matter how much moisture is present. When the moisture is less than 30%, the strength increases as the moisture decreases. Oven dry wood may be as much as 4 times as strong as the same wood containing 30% or more moisture.

2.2.14 Sappi – A brief history

In December 1936, the South African Pulp and Paper Industries Limited was registered as a company with an authorised capital of GBP750,000 (ZAR1,5 million). In 1947, the company purchased two farms north of the Tugela river in Zululand with the aim of establishing a paper mill. Three years later, the mill was named Tugela. In 1954, Tugela mill produced its first reel of paper for Kraft packaging.

The company continued to grow and in 1962 produced its first millionth ton of paper. A year later, the Tugela mill purchased a No 2 machine to specialise in Kraft linerboard.

In 1973, the company re-registered as Sappi Limited. Since then, Sappi has become established on the world market: it is one of the most global paper companies with 20 mills around Europe, North America and Southern Africa. Sappi is the world's largest producer of coated fine paper, has the fastest growing sector in the paper industry and leads market shares in Europe, North America and Europe.

2.3 Modelling of the Kraft digester

2.3.1 Some background

The pulp and paper industry has three major challenges. The first and probably the most important is the capital intensive aspect of this branch of industry. Secondly this industry utilizes a raw material which is a natural product with its non-uniform characteristics and behaviour. And finally, it has to deal, as with any other industrial operation, with an increasing environmental responsibility exacerbated by the exploitation of a natural raw material.

Hence, rigorous engineering approaches should be employed to reach and maximize when possible the return from capital investments. The natural aspect of the raw material highlights the fact that nature cannot be tampered with. Over the past twenty years, the industry of pulp and paper tried to implement new scientific and engineering approaches to fill the gaps in our understanding of the manufacturing steps. This attitude also tackles the third challenge and entices industry to improve its accountability for environmental issues.

Process control is essential in the pulp and paper industry to achieve the goals proposed by these challenges. It has reached a certain level of importance over the past two decades. The pulp and paper industry shares a lot in terms of unit operations with other processes in petroleum and chemical industries. So far, selected process control approaches have been established in the pulp and paper industry. However, the challenges imposed on the pulp and paper industry include the stochastic nature of the raw material, the long time delays, the incomplete measurements and the multivariable process behaviour.

Vroom (1957) expressed the first digester modelling using the H-factor. Vroom's work is known as the Purdue model, a reference to the Purdue University. This factor combines time and temperature effects in a single variable, assuming a first order mechanism. In 1973 and 1984, Hatton correlated numerous batch cooking experiments to propose a universal empirical relationship for Kappa number. These models were really specific to some aspects of digesters. Fundamental approaches started with Smith and Williams (1974) then Christensen, Albright and Williams (1982) and Butler and Williams (1988).

A combination of transport and kinetic relationships between the three phases of the digester was used to describe the operations of the continuous digester: wood chips, entrapped liquor and free liquor. The model incorporates different zones where the chips and free liquor evolve: co-current and counter-

current. Gustafson et al. (1983, 1984) and Agarwal, Gustafson and Arasakesari (1994) developed another fundamental model with particular attention to the diffusion effects of liquor in chips.

But digesters are still mysterious in some ways. The delignification reactions are assumed from estimations. Model developers rely on laboratory and mill data to adjust their parameters and confirm their choices. Thus, some improvements are made constantly to get the best accuracy on the models: Harkonen (1987) developed a model for the chip compaction problem concerning the two-phase flow system. Datta et al. (1994) simplified and improved the reaction kinetics. Recent work takes into account the latest design developments present in the new installations, and tries to target models for dynamic analysis, model reduction and robust controller design: Funkquist (1995), Michelsen (1995), Wisniewski (1995) and Kayihan et al. (1996).

According to what has been said in Chapter 3, digesters present some interesting characteristics. One of the major concerns during pulp manufacturing is to keep chip levels constant in the digester and if present, in the impregnation vessel. Belanger et al. (1986), Petrus (1990) and Allison, Dumont and Novak (1991) have developed and implemented a self-tuning approach for this matter based on generalised predictive control.

Kappa number control is *the* problem for digesters. This value is affected by a number of variables, all inherent in the digester: the raw material, the variation in the feedstock, the long response time. Usually, manual adjustment is the key to solve the problem. Unfortunately, the reaction to this adjustment can take several hours and can also interact with other adjustments. Then, the traditional way is to be quite conservative and leave the values as they are.

However, the benefits of automation have been revealed in a number of applications. For the last ten years, on-line measurements and adjustments made it possible to get a better overall view of the process and to obtain better results. Some methods have been developed for batch digesters and could possibly lead the way for continuous digesters.

Advanced control applications use a simplified reference model for Kappa number predictions and update model parameters on-line with each measurement or as needed: Beller et al. (1988) developed a simple two-dimensional model using temperature input and effective alkali to predict Kappa number and residual alkali. Christensen et al. (1990) and Michaelsen et al. (1994) used a simple mechanistic model compensated by an optimal state estimator as the basis for a model predictive control algorithm. The opportunities of improvement are far from being exhausted.

The Purdue model, one of the first models developed for Kraft process, represents a solid base for numerous models developed later. This model assumes that 5 wood species concentration states are enough to describe the digester: high reactive lignin, low reactive lignin, cellulose, galactoglucomannan and arabinoxylan. These 5 states are supplemented with the concentration of hydroxide ion and hydrogen sulphide ion. Actually, this gives us 7 states. Of these 7 states, the hydrogen sulphide ion concentration can be considered constant and the hydroxide ion concentration can be computed from a stoichiometric balance or even can be measured online and then be considered as an input in the form of a measured disturbance.

Numerous works have been completed based on the Purdue model: Wisnewski, Doyle and Kayihan (1997), Doyle and Kayihan (1999).

Gustafson et al. (1983) developed a model where the wood components are divided into two (and not five like in the Purdue model): lignin and carbohydrates. The kinetics are here divided into three periods: initial, bulk and residual (Figure 2-14). This model is called the 3-stage model.

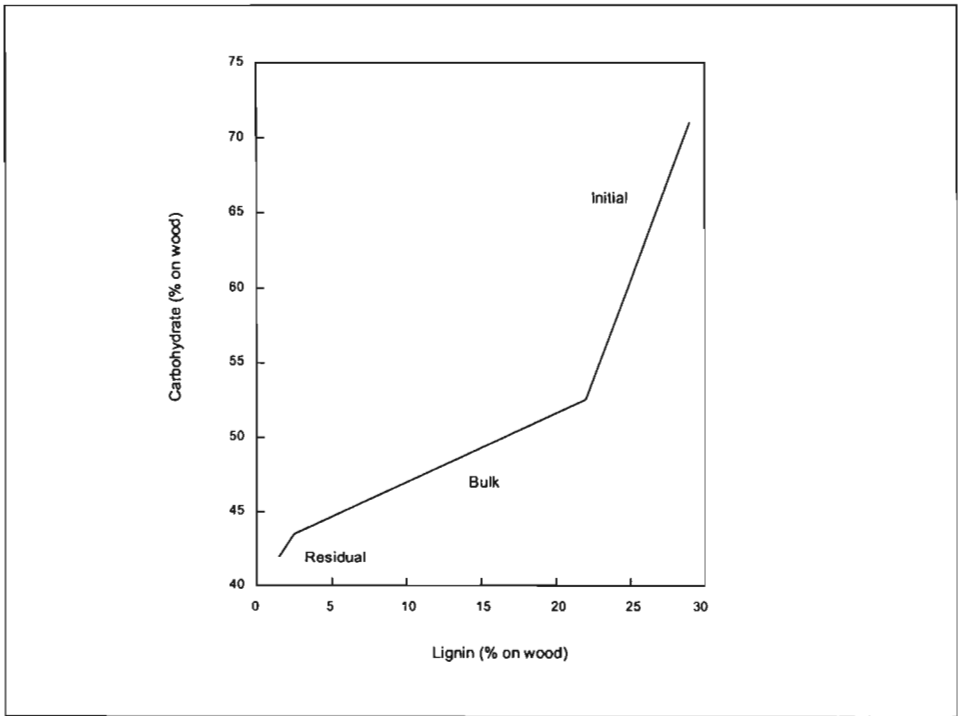


Figure 2-14. Carbohydrate yield as a function of delignification showing 3 distinct periods (Smook, 1994)

Gough and Kay (1996) implemented Dynamic Modelling Technology in their control scheme. This structure solves the problems encountered by using a Smith Predictor: long development time, repeated tuning and poor reliability. They mainly focus on the relation between effective alkali and

Kappa number. Effective alkali control is a problem in the feed-forward structure as this parameter is sensitive to chip quality variations. Chip moisture for example can vary from 40 to 60% in a single day of production. From an economical point of view, this method aims at reducing costs while reaching the Kappa number wanted.

Kayihan (1998) proposed an intuitive control approach and compared the performance obtained to a conventional feed-forward scheme. Using three Kappa numbers to indicate the progress of reactions along the digester, a 5*5 unconstrained MPC structure was developed and tested. Kayihan showed that controlling the reaction profile of the digester is much more effective than just controlling the blow-line Kappa number. Of the three Kappa numbers, one was physically available for measurement while the two others had to be estimated. This method is more likely to offer consistent fibre properties.

Wisniewski and Doyle (2001) compared three model predictive controllers, each incorporating internal models with varying degrees of complexity, on a continuous digester. They use a linear state-space model for the first two models and a nonlinear fundamental model for the third one.

This study utilized a digester similar to an industrial one. The first MPC rejects stochastic composition disturbances but offers significant deviations in the closed-loop Kappa number. The second MPC reacts perfectly when it comes to rejecting the stochastic disturbances. The variance is approximately the same as the measurement noise on the Kappa number signal. The third model's performance was about the same as the linear MPC's however it was superior for deterministic disturbances.

Kayihan (2002) incorporated a grade transition with dynamic compaction in packed beds of chips and the transport/convection effects affected by chip size distribution. The real challenge does not come out on how to include these variables in the model but more from the considerable number of equations representing the dynamic behaviour. This new generation of model was developed to provide high fidelity simulation abilities.

2.3.2 Development of a mathematical model

Two different approaches can be used to design a controller:

- Experimental approach: the physical equipment of the process is known. Consequently, the designer changes the values of different inputs and observes how the corresponding outputs react with time. This modus operandi is time and effort consuming as a number of experiments need to be achieved.

- Theoretical approach: quite often, the design of a control system needs to be done before the process has been constructed. This method relies on mathematical equations developed to represent the dynamic behaviour of the chemical process.

In the present work, concern was with a model which could provide feedback for a controller. A mathematical model was sought to represent the digester. Furthermore, the mathematical modelling could have benefit from a financial point of view. Indeed, physical experiments to adjust the final product, pulp in our case, would require a very comprehensive measurement set, which could lose accuracy as time passes.

2.3.3 Feedback control of systems with large dead time

The process of Kraft pulping involves a long response time as we saw earlier. In such a situation, a conventional feedback controller would provide unsatisfactory closed-loop response for the following reasons:

- A disturbance entering the process will not be detected until after a significant period of time
- The control action that will be taken on the basis of the last measurement will be inadequate because it attempts to eliminate an error that originated a while back in time.
- The control action will also take some time to make its effect felt by the process.
- As a result, significant dead-time is a source of instability for closed-loop responses.

Smith was the first one to propose a solution to reduce the effect of dead-time in classical feedback controllers, known as the Smith predictor (Smith, 1957).

The Purdue model fits the measured data for the modern cooking schemes quite well. It has the advantage that it describes the kinetics with respect to hemicellulose which are needed for the pulp property predictions. However, high-running costs of industrial scale digesters, difficulties in sampling and the large time lags make it necessary to work with laboratory studies and modelling tools to correlate pulp properties with operating conditions to obtain a relevant model for a specific plant.

A detailed physical representation of the actual process would require:

- A description of the chemical kinetics and diffusion at the chip scale
- A description of the flows within the digester
- A description of the external configuration and auxiliary control schemes

2.4 Smith prediction

Time delay is a very common phenomenon encountered in the processing industries. It causes major difficulties in the design and implementation of control. The presence of time-delay in a feedback control loop could be a severe hindrance to good process operation. The idea of the Smith predictor (Smith, 1957)(Figure 2-15) is that a model can predict the process variables before it is possible to measure these variables. So, when the appropriate measurement becomes available, the error, synchronised from a buffer file, is used to correct the current model predictions. If used in closed loop control then we get an Internal Model Control (IMC) (Garcia and Morari, 1982). Smith predictors have been used in many areas since. Its performance is superior to the conventional proportion-integral-derivative (PID) controller alone in both set-point and regulation responses.

The Smith predictor has been extended to many applications. It has been tuned for multivariable systems with single delay (Alevsakis and Seborg, 1974) and with multiple delays (Ogunnaik and Ray, 1979; Ogunnaik *et al.*, 1983). The Ogunnaik approach is represented in Figure 2-16.

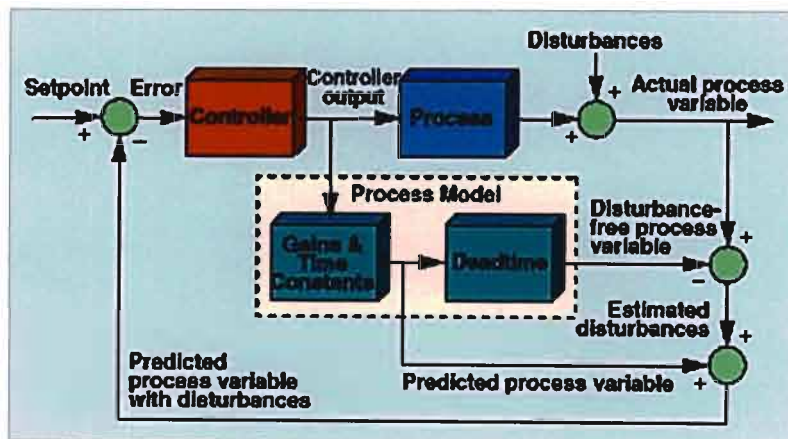


Figure 2-15: The mathematical model of a Smith Predictor (VanDoren, 1996)

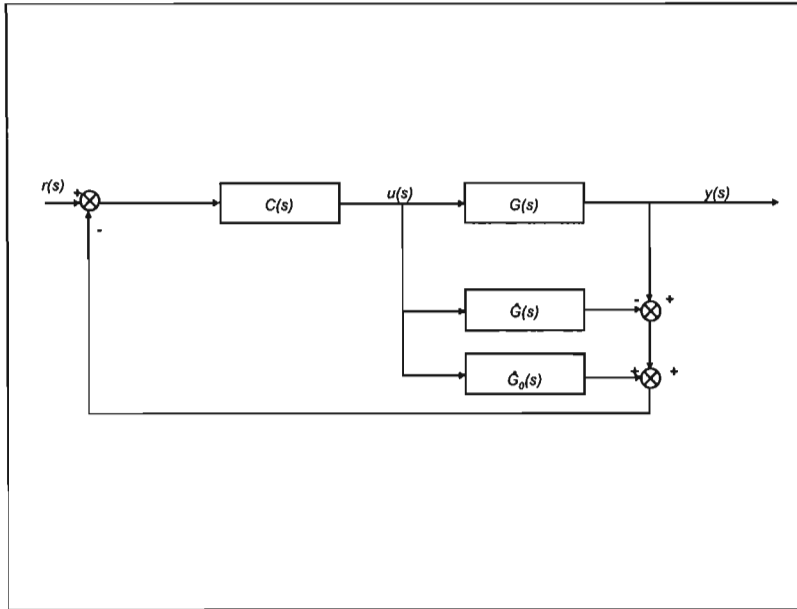


Figure 2-16: Multivariable Smith Predictor Structure (Ogunnaike, 1979)

To avoid the mismatch effect caused by inaccurate modelling in the Smith predictor, the use of adaptive techniques is desirable, Isermann (1982) and Bahill (1983). Habermayer and Keviczky (1985) added on-line adaptive estimation of a varying dead-time lag. Although all the tools, both the hardware and the software, were available for developing adaptive modelling, studies took some time before being presented or implemented. This delay might be attributed to the fact that the Smith predictor needs the exact models of both the delay-free and the time-delay part of the process.

We will illustrate the Smith predictor with a first-order lag process with dead time D:

$$G_{M(s)} = \frac{K_p e^{-Ds}}{\tau_p s + 1} \quad (2.2)$$

where K_p is the gain, τ_p a time constant and D the delay.

In a control loop, it is a special type of model-based controller, in the same family as internal model control (IMC). The overall open-loop process is G_M .

$$G_M = G_{ND} e^{-Ds} \quad (2.3)$$

where G_{ND} is clearly the non-delay part of the open-loop transfer function (Figure 2-17).

If a conventional feedback controller B is used, the closed-loop is:

$$X = \frac{BG_{ND}e^{-Ds}}{1 + BG_{ND}(1 - e^{-Ds})}(X_{set} - X) \quad (2.4)$$

where X is the process variable and X_{set} its setpoint.

The existence of the dead time will force the controller to be detuned to maintain closed-loop stability. Using the Smith predictor (Figure 2-18), the closed-loop characteristic equation is changed.

$$\frac{M}{E} = \frac{B}{1 + BG_{ND}(1 - e^{-Ds})} \quad (2.5)$$

Considering the outside loop, we have

$$X(1 + BG_{ND}(1 - e^{-Ds})) = BG_{ND}e^{-Ds}(X_{set} - X) \quad (2.6)$$

$$X(1 + BG_{ND}) = BG_{ND}e^{-Ds}X_{set} \quad (2.7)$$

$$\frac{X}{X_{set}} = \left(\frac{BG_{ND}}{1 + BG_{ND}}\right)e^{-Ds} \quad (2.8)$$

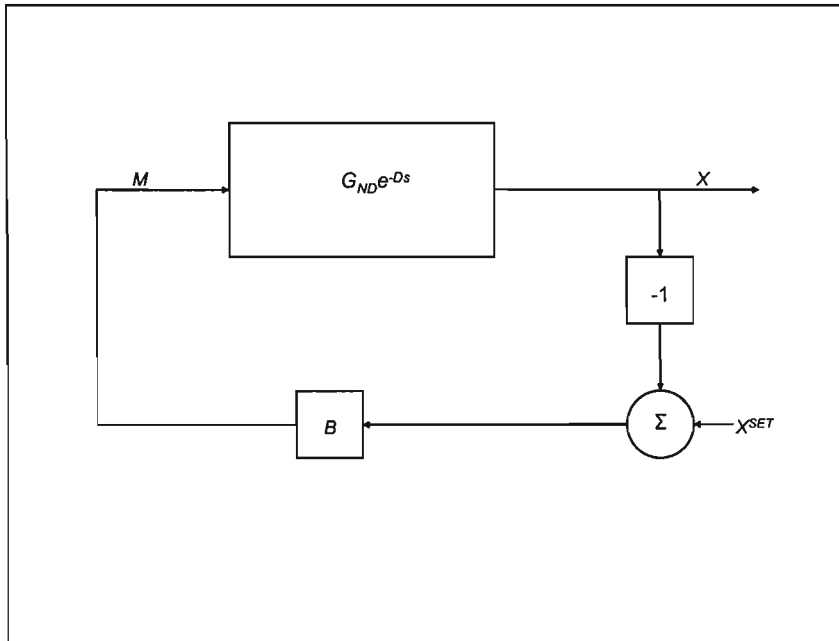


Figure 2-17: Smith Predictor a) Normal (Ogunnaike, 1979)

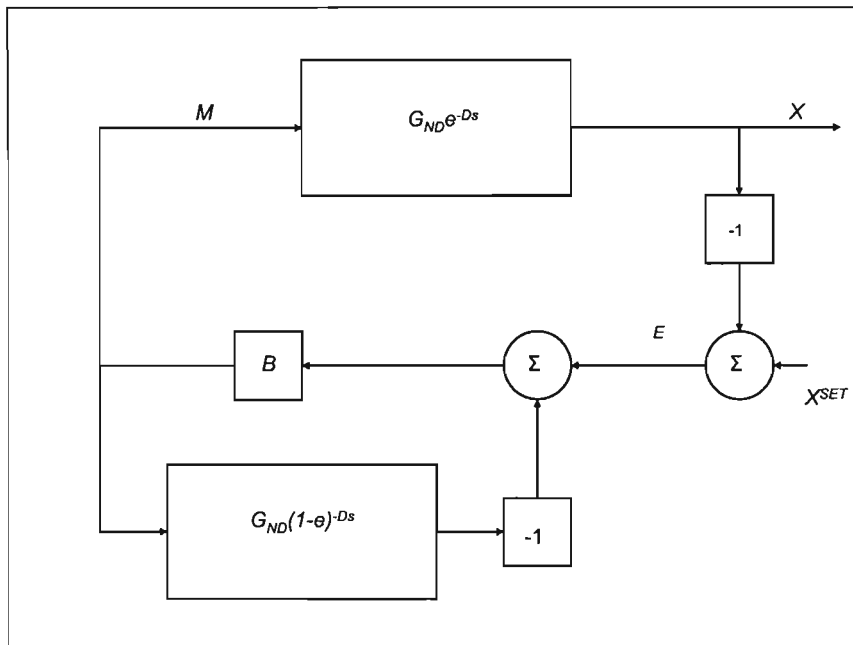


Figure 2-18: Smith Predictor b) Predictor (Ogunnaike, 1979)

Solving for the closed-loop, the transfer function is

$$\frac{X}{X_{set}} = \frac{BG_{ND}}{1 + BG_{ND}} e^{-Ds} \tag{2.9}$$

Notice that the dead-time lag has disappeared from the denominator, thus strongly affecting stability via the characteristic equation.

A closed loop incorporating a Smith predictor includes two simulators of the plant as we saw: the one concerning the whole plant and the one of the delay-free part. To function correctly, they need to reproduce the plant behaviour perfectly. But this hypothesis can not be assumed for sure because of plant uncertainty. Then, plants are controlled by “mismatched” controllers. Smith predictors work well in the case of perfect matching though (Yamanaka, 1987).

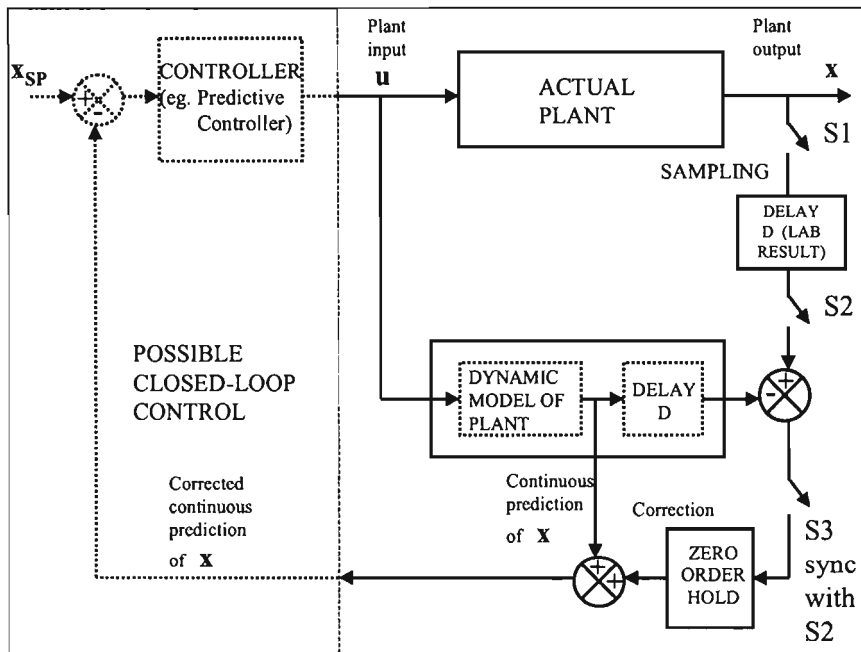


Figure 2-19: Scheme for prediction of Kappa number with intermittent correction synchronised by a Smith Predictor. Possible closed-loop control completes an "Internal Model Control" format (Mulholland, 2002)

Gough and Kay (1996) remark that the main difficulties of continuous pulp digester control are the long dead-time and varying conditions. They developed a “Dynamic Modelling Technology” (DMT) approach to this problem using an adaptive model predictive controller. Their model was based on

orthonormal Laguerre functions following the techniques of Dumont and Zervos (1986). One advantage of this type of model is that the Laguerre functions represent (varying) dead-time accurately. In contrast, it is not possible to adapt the dead-time in standard Dynamic Matrix Controllers. The authors note that optimal control of a digester aims to achieve maximum pulp production at a specified Kappa number, with a minimum of chemicals and energy input.

Kayihan (1998) notes that the control of continuous digesters, expressed as a reaction profile control problem, is similar to the previous methods for distributed parameter plug flow reactors.

The adaptive Smith predictor uses a single sampling rate: the controller output and the parameter estimator are updated at the same frequency. Furthermore, a large sampling period is suggested as a reduced order model can be used with a good degree of robustness in approximation and shows more stability (Aström, 1984).

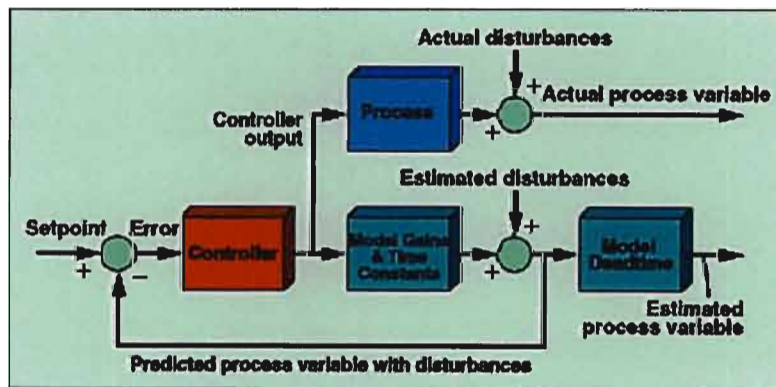


Figure 2-20: Effective removal of dead-time (Van Doren, 1996)

Figure 2-20 is similar to Figure 2-15 with the blocks rearranged. It also shows an estimate of the process variable (with both disturbances and dead-time) generated by adding the estimated disturbances back into the disturbance-free process variable. The result is a feedback control system with the dead-time outside of the loop.

The Smith Predictor essentially works to control the modified feedback variable (the predicted process variable with disturbances included) rather than the actual process variable. Assuming the Smith Predictor is successful and the model matches the process, the controller will simultaneously drive the actual process variable towards the set-point whether the set-point changes or a load disturbs the process.

Unfortunately, those are assumptions. It is easier for the controller to meet its objectives without dealing with the dead-time, but it is not always a simple matter to generate the process models needed to make the strategy work. Even the slightest mismatch between the process and the model can sometimes cause unstable operation. There have been several fixes proposed to improve on the basic Smith Predictor, but dead-time remains a particularly difficult control problem.

2.4.1 Internal model control (IMC)

Internal model control is becoming more and more popular in the chemical processing industries. The structure of the internal model control incorporates an explicit model of the plant and has been shown to be very effective for the control of plants. However, a control scheme based on the IMC structure needs the availability of a fairly accurate model of the plant, to be used as part of the controller.

One technique developed to get a more accurate model of the plant is adaptive parameter estimation. This technique is used when the model of the plant is well known but when plant measurements are the major uncertainty.

2.4.1.1 MPC

Model predictive control involves computation of the control input at a certain time by using a model of the plant to predict future values of the output over a finite time horizon. The next step will be to choose the right control input to minimize the overall cost to reach the predicted output. Cost is usually a quadratic function that penalizes:

- The deviations of the predicted output from the desired values
- The control effort required

The calculated control input is then applied over a time horizon that can be less or equal to the time horizon over which the cost function was minimized. Following values of the control input are obtained by repeating this procedure.

2.4.1.2 IMC

The controller scheme shown in Figure 2-20 is referred to as the internal model controller structure. When constraints on the process variables are ignored, a linear time-invariant controller can be obtained. Garcia and Morari showed that most unconstrained model predictive controllers could be implemented as shown in Figure 2-20 (Garcia and Morari, 1982).

If $G(s)$ is stable and $G_0(s) = G(s)$ then the structure is stable if and only if the transfer function $C(s)$, usually named the “IMC parameter” is stable. That is to say that if we start with an open loop stable plant and use an exact model in the IMC design, then the closed loop system will continue to be stable as long as the IMC parameter is chosen to be stable.

Unfortunately, it is not possible to get the two functions $G(s)$ and $G_0(s)$ exactly identical. Thus, there is no guarantee of closed loop stability. Designing the IMC structure would then need to account for the mismatch. Two widely used techniques are robust control and adaptive control.

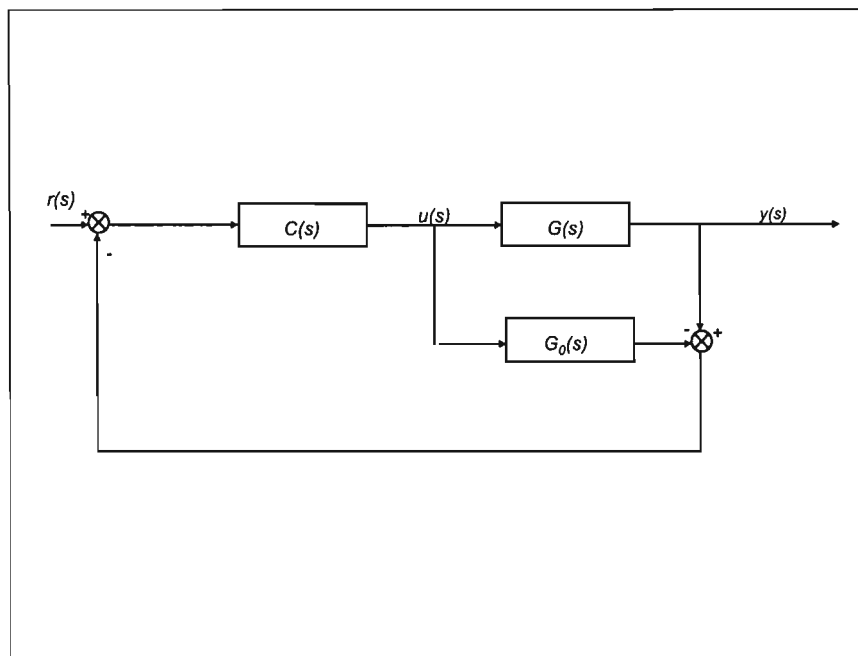


Figure 2-21: The IMC configuration

2.4.2 Robust control

In robust control, one seeks to design a single time-invariant controller that can assure that the closed loop system holds its desired characteristics despite modelling errors such as plant model mismatch. Since the errors are unknown, it is customary to consider classes of error that are encountered in practice. Some of these classes are listed below:

- Multiplicative perturbations
- Additive perturbations
- Stable factor perturbations
- Parametric uncertainty

- Disturbances and noise
- Mixed type uncertainty

2.4.3 Adaptive control

Adaptive control is suitable when the plant uncertainty is predominantly of the parametric type and is too large to be handled using a single fixed controller. One can estimate on-line the transfer function of the modelled part of the plant and design the IMC controller according to these estimates. But since the parameter estimate will change with time, the controller will no longer be time invariant. Furthermore, the closed loop will be nonlinear and time varying, thus needing some more complex analysis.

Gough and Kay (1996) presented the DMT adaptive control (Figure 2-22). The advantage of the DMT structure is that, contrary to other schemes that require a detailed knowledge of the transfer model, it doesn't necessitate a predetermined model of the process to be controlled. It forecasts the process response so that the set point is attained as quickly as possible with little or no overshoot, using a minimum of control effort (actuator manipulation).

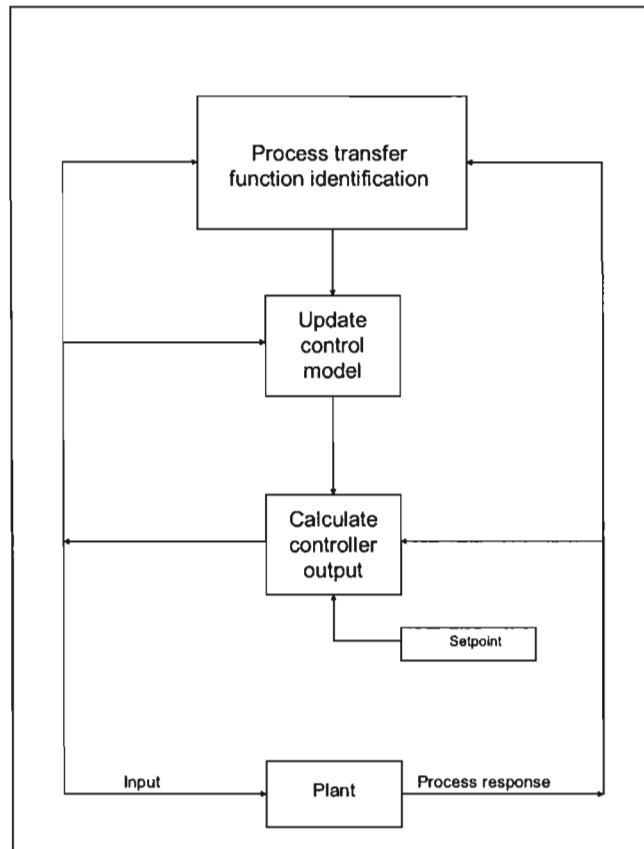


Figure 2-22: Basic steps in the DMT controller

- 1- Process transfer function identification: the process model is adjusted by relating observed process responses to past control actions
- 2- Control update: the previous control action is taken into account to produce a new prediction of future process response
- 3- Control output: the predicted process response is used to calculate the required controller output to bring the process variable to the desired set point with minimum control effort

2.5 Different models

As stated previously, the Kraft digestion is of paramount importance and many mathematical models were established in the past. Most of these models relate the Kappa number to the variables affecting it: sulfidity, effective alkali, moisture content, variation in wood type and H-factor. The H-factor is the relationship between time in the reactor and temperature in the reactor and effective alkali. This variable is said to be the most crucial factor amongst all.

Some fairly acceptable assumptions can be made to facilitate the calculations.

- moisture content is constant
- wood properties do not vary (same type of wood)
- sulfidity is controlled
- chemical charges are constant

It would be normally attempted to differentiate the types of wood as they have different characteristics. Nevertheless, the Sappi Tugela mill does not take into account these differences. We discuss the variables later in Chapter 4 and how they can influence the results of the modelling.

2.5.1 Method of Kerr

A study by Russel (1996), on the Sappi Ngodwana Mill, which uses the same kind of digester as in Tugela Mill, led to a model (with changes made by Sappi). This model is determined by the equation (2-10):

$$L_{final} = \frac{(K - 1.6)(0.54K + 315.4)}{686(7.29 - 0.0106K)} \quad (2-10)$$

Where L_{final} represents the final rate of delignification of the pulp and K the Kappa number.

2.5.2 Method of Edwards-Nordberg

This model is described by equation (2-11):

$$K * Y = 0.14286 \frac{6.15 \times 10^7}{\left(\frac{S}{2-S}\right) \left(\frac{EA_{charge}}{Lw}\right)^2 H} \quad (2-11)$$

Here Lw represents the liquor to wood ratio, S the sulfidity and Y the pulp yield. H is the H-factor and EA_{charge} is the effective alkali charge (weight % as Na_2O on wood).

2.5.3 Method of Hatton

Hatton (1973, 1976) presented results obtained from a series of tests on different softwood and hardwood pulps. The equation (2-12) gives the Kappa number:

$$K = A - B(\log H)(EA^n) \quad (2-12)$$

Where A , B and n are constants for a given wood species.

K = the total pulp yield (%)

H = H-factor

EA = the applied effective alkali charge (weight % as Na_2O on wood)

2.5.4 Discussion

Sappi was using Kerr and Edwards-Nordberg models for its Ngodwana mill. It is important to note that the model in Equation 2-11 is the one used by Sappi with some changes from the original model. Indeed, the value 0.14286 is an adjustment from the model given by Edwards and Norberg (1973).

The Method of Hatton is interesting but needs some extra work based on the fact the different constants (A , B and n) for each wood species concerned must be established before the data treatment. This implies that the wood feedstock is known and will not vary in time. The Sappi Tugela mill wood feedstock is composed of hardwoods and softwoods where the distribution is unknown. This would inevitably create errors in the model.

The Kerr model and the Edwards-Nordberg model give satisfactory prediction results (Figures 2-23 and 2-24) as the calculated and measured Kappa numbers are compatible. But these correlations are not to be used for high Kappa number as the model does not give correct figures. Indeed, it can be seen that for Kappa numbers above 100 the models do not give realistic values.

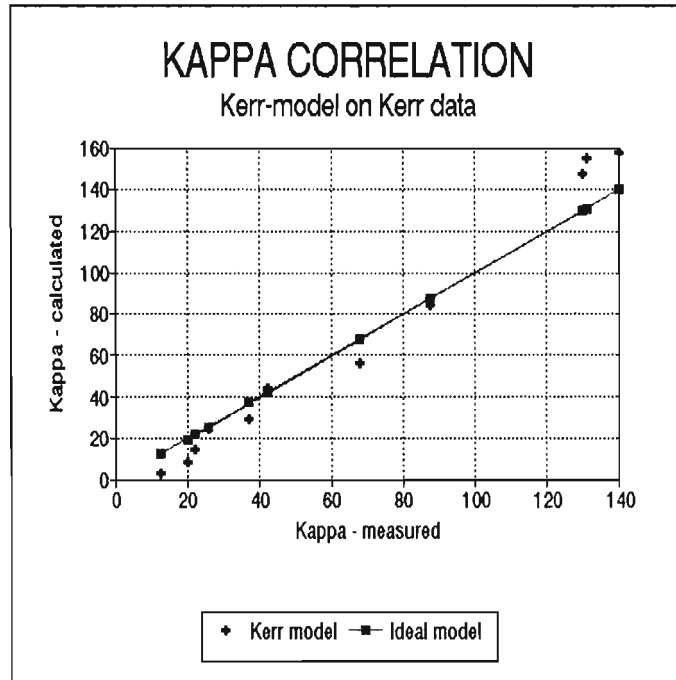


Figure 2-23 : Sappi-modified Kerr model fit to Kerr data (De Vaal, 1996)

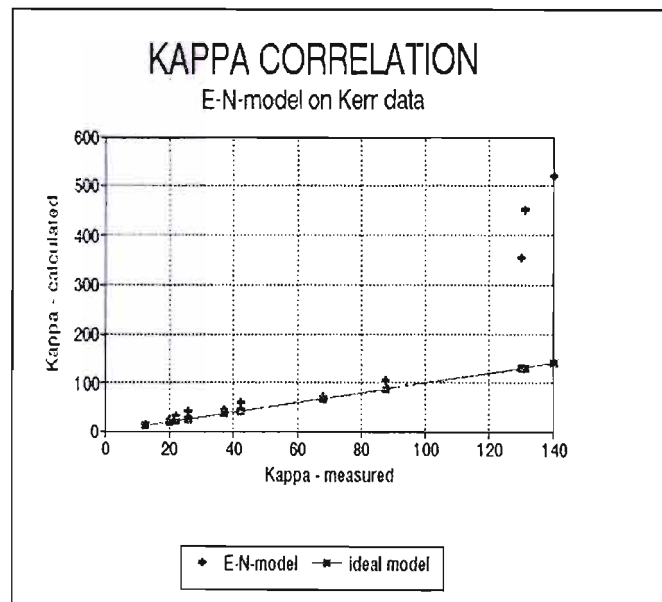


Figure 2-24 : Edwards-Norberg model fit on Kerr data points (De Vaal, 1996)

It is also important to note that many models developed so far used batch digesters to recreate the mill environment. Continuous digesters have a different behaviour and such models should be employed with care.

De Vaal (1996) suggested in his study that a “simple model for estimating Kappa number be used, relating only H-factor to Kappa number. This should work well provided that the other parameters influencing Kappa number are kept under closed loop control. As more reliable data becomes available, the model can be expanded to include effects of the other factors”. This way of proceeding concurs with the one described in this study.

CHAPTER 3

Modelling Approach Used In This Study

Once the process had been examined and a literature review done, the scheme of the model to be developed was decided: it would be a simple, yet robust model, based on the principal parameters of the digester. The most important variables were noted and isolated for further investigation.

The plant staff keeps an electronic version of the digester parameters. They record the main variables every two hours. A routine laboratory analysis gives the Kappa number. This result is delayed but the operators can get an idea of the present process operation from it and correct some parameters if necessary.

A Smith predictor was proposed early in the project. Indeed, the long delay in the digester itself makes it clear that dead-time plays an important role in the process. Such an intelligent observer would allow earlier feedback.

The Kraft process, as we saw for the chemicals recovery (refer to Chapter 2), includes numerous recirculation cycles. These re-circulations make the process complex.

3.1 First step: data collection

The data collected from the mill was chosen based upon some basic criteria: the process should be settled for a few days, the longer the better, and the product pulp should be of a good quality. Once we had these two conditions, then the data collection was initiated.

3.1.1 Data treatment on Excel & Matlab

3.1.1.1 Matlab presentation

MATLAB, which stands for MATrix LABoratory, is an interactive software package for numerical computations and graphics. Founded in 1984, The MathWorks released the first edition 15 years ago. Many designers of embedded control systems rely on this product and around 500,000 of the world's leading technical people have adopted this program.

Because the syntax for using MATLAB interactively is the same for writing programs, a code can be quickly converted into a reusable, automated analysis routine. Unlike most traditional languages, MATLAB gives the freedom to focus on technical concepts rather than on programming details like memory management and variable declarations. Furthermore, M-files require no compiling or linking, which allows editing and step-by-step debugging of a program without having to leave MATLAB.

3.1.1.2 Data treatment

The sets of plant data are issued for each month. By accumulating these, a long period of operation can be examined. Once the desired parameters are isolated on an Excel sheet, they are re-organized according to their importance. Indeed, the days of non-production, where all or almost all the parameters are set to 0 are useless for the mathematical model. A small program has been established under Matlab to avoid such gaps. In fact, selected missing parameters in the data collection might also occur. The subroutine is used to interpolate these missing values.

05/12/2001	1:00	112	130	136	133	2850	4800	7.5	52.5	0:00	78
	3:00	111	133	126	132	2900	4900	7.5		2:00	80
	5:00	111	130	126	132		4884	7.5	51.2	4:00	81
	9:00								53.3	8:00	82
	11:00	111	137	134	132	2880	4670	7.6		10:00	78
	13:00								51.7	12:00	77
	17:00								55.3	16:00	80
	19:00	112	131	136	133	2867	4901	7.5		18:00	81
	21:00	112	131	137	131	2880	5150	7.5	52.9	20:00	80
	23:00	111	138	135	131	2849	4951	7.5		22:00	82

Figure 3-1 : Some parameters taken from a set of data.

We can clearly see in Figure 3-1 that on this set of data, some cells are empty. This reflects well the digester behaviour as the process is not continuously running: downtimes occur as well as manufacturing problems, leaving no data. This is where the program is important. Let us say we miss the value at a time t : the Matlab subroutine will take the previous value available, for example $t-1$, and the next available value, $t+1$, and make a linear interpolation to obtain the missing value. This subroutine allows one to obtain a continuous set of data, which is important for analyzing the digester which has a residence time of 6 to 12 hours.

3.1.2 Calculations

Once the subroutine has been run on the set of data, a linear regression is performed to express the Kappa number in terms of a linear combination of key variables and a bias. The Kappa number is obtained from the laboratory analysis. This analysis occurs every two hours. It presently allows the operators to obtain a feedback on the settings used on the digester. The two hours delay is taken into account in preparing the regression data set. The regression itself is easily performed using a standard linear regression function such as is available in spreadsheet programs.

For a particular set of regressed coefficients, we calculate our prediction of the Kappa number for the same data records. This predicted Kappa number is then compared with the measured Kappa number.

Once plotted, the two trends look like the graph in Figure 3-2.

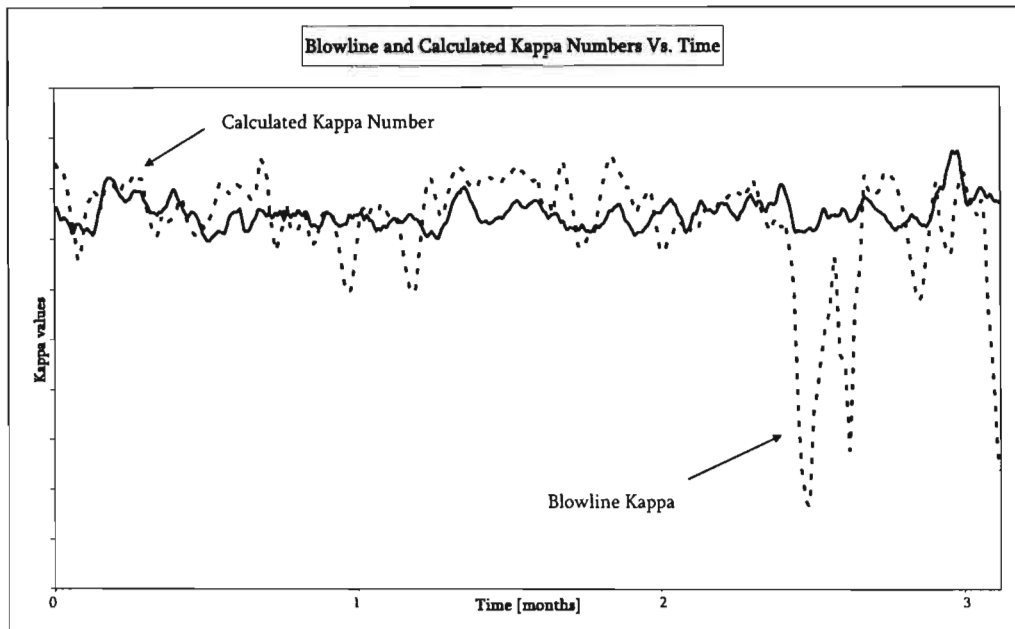


Figure 3- 2 : Blowline and calculated Kappa numbers vs. time

3.2 Second step: Going On-line

3.2.1 Creating a Graphical User Interface (GUI)

A GUI is a graphical user interface on a computer. The term came into existence because the first interactive user interfaces on computers were not graphical; they were text-and-keyboard oriented and usually consisted of commands you had to remember and computer responses that were infamously brief.

Today's major operating systems provide a graphical user interface. Applications typically use the elements of the GUI that come with the operating system and add their own graphical user interface elements and ideas. Elements of a GUI include such things as: windows, pull-down menus, buttons, scroll bars, iconic images and the mouse. With the increasing use of multimedia as part of the GUI, sound, voice, motion video, and virtual reality interfaces seem likely to become part of the GUI for many applications. A system's graphical user interface along with its input devices is sometimes referred to as its "look-and-feel."

The GUI familiar to most of us today in either the Mac or the Windows operating system and their applications originated at the Xerox Palo Alto Research Laboratory in the late 1970s. Apple used it in their first Macintosh computers. Later, Microsoft used many of the same ideas in their first version of the Windows operating system for IBM-compatible PCs.

From an industrial point of view, the GUI allows operators to manipulate the plant in a user-friendly environment. More and more companies use this system to control their processes: indeed, you have a global view of the processes with the parameters needed. It seemed normal to have a GUI of the Kraft observer model along with all the utilities already in position at Tugela. This was facilitated by the installation of a Distributed Control Systems (DCS) concerning the two lines of production at Tugela.

The Distributed Control Systems' goal is to spread computing and controlling functions throughout the plant. It is preferable to use smaller computers in place of a large and complex one. As numerous mini-computers are deployed on different tasks, it is easier for operators to interact with them. Usually two operators take care of the plant. One operator is on the ground, in constant radio communication with the operator in the control room, in front of the DCS console. The latter gives indications to the operator in the field, directing his actions to improve the process.

3.2.2 The Sappi Tugela GUI

In the 1960's, the digital computer was first used in process control. This introduction was made cautiously because of the high capital investment. In the 1970's, with the development of mini-computers and the decreasing cost, it became much easier to justify and install computing systems in control rooms.

The GUI created for the project is very simple and has all the features needed. First of all, as it's based on the DCS, we can gather all the parameters needed as almost all the major parameters of the digester are listed in the DCS. Then, as the DCS refreshes all the parameters every second, it is easy to build up longer term averages if necessary. The main part of this GUI is the implementation of the model created for the project. The model is fairly simple and does not require a lot of resources.

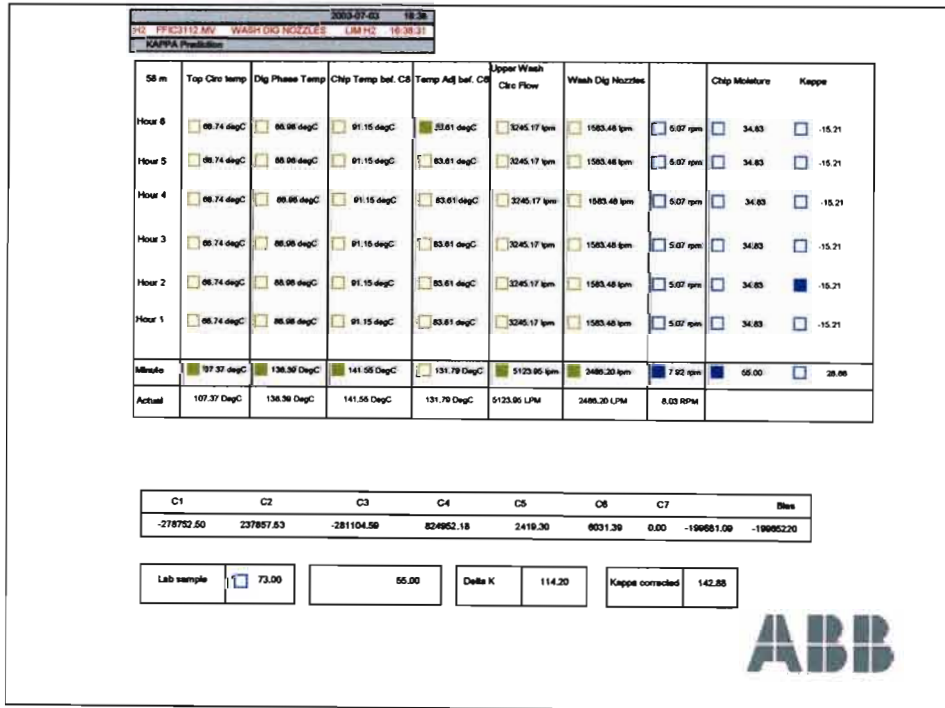


Figure 3-3 : The first GUI

The first GUI (Figure 3-3) was created to test the model directly. It allowed performance of basic operations and validation of the concept. The second GUI was created some time later (Figure 3-4).

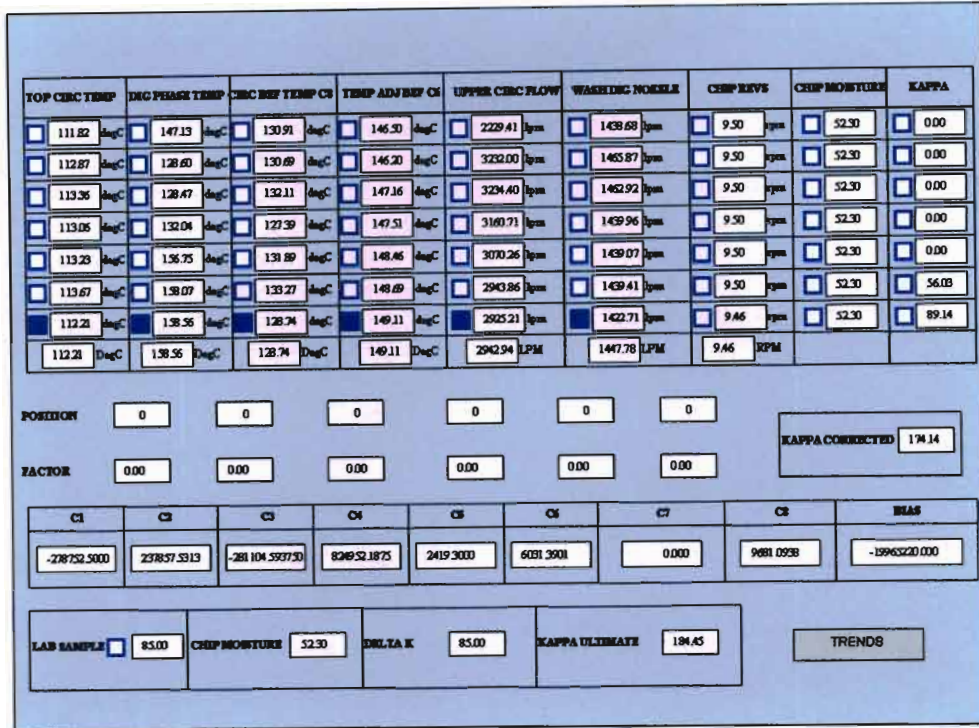


Figure 3-4 : The second GUI

As presented in Figure 3-4, the GUI is separated into different sections. The upper part of the window is dedicated to the general DCS operation, including the black window which is reserved for the alarms.

The bottom part gathers the parameters the operator can enter into the model (Figure 3-5).

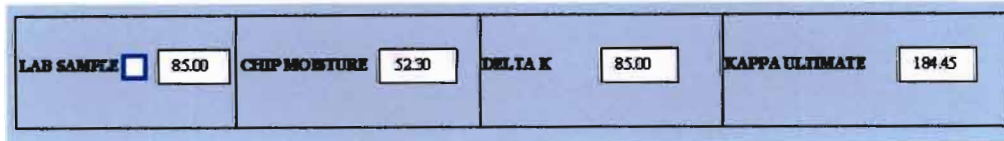


Figure 3-5 : GUI- the bottom part

The lab sample on the far left can be set according to the laboratory analysis made every two hours. As for the Chip Moisture, it was decided to keep it constant as there are infrequent laboratory analyses available. The value can also be entered by the operator. The last two figures represent the “deltak”, the difference between the Kappa number actually calculated and the Kappa number from the lab sample. The “Kappa corrected” is the prediction of the present Kappa value leaving the digester. The “Kappa ultimate” is the final value: if present plant settings are maintained.

The coefficients for the linear model used are entered manually by the operator. The section of the GUI dedicated to this operation is shown in Figure 3-6.

C1	C2	C3	C4	C5	C6	C7	C8	BIAS
-28752.5000	239857.5313	-281.104.599730	824952.1875	2419.3000	6031.3901	0.000	9681.0938	-19965220.000

Figure 3-6 : GUI- the coefficients

In the Figure 3-6, we can see the coefficients needed for the model to function correctly. They are named C1 to C8. As we are using a linear equation, a bias is necessary. Its value is located at the right far end of the figure. These coefficients are manually entered. To do so, the operator just needs to click on the coefficient he wants to set: another window will pop-up, asking for the value. Once all the values are correctly set, they are memorized into the model’s program code until the operator changes them, after an update of the model for example.

You can notice that the value C7 is set to 0.0. This coefficient is reserved for the Chip Moisture. After analysis of its variations, it was found that the value does not require a coefficient for the time being, because no correlation was detected with it.

Finally, Figure 3-7 depicts the GUI of the model. There is one column for each measurement used by the model.

TOP CHRC TEMP	DEC PHASE TEMP	CHRC REF TEMP C8	TEMP ADJ REF C1	UPPER CHRC FLOW	WASHING NOZZLE	CHIP REV'S	CHIP MOISTURE	KAPPA
<input type="checkbox"/> 111.82 degC	<input type="checkbox"/> 147.13 degC	<input type="checkbox"/> 130.91 degC	<input type="checkbox"/> 146.30 degC	<input type="checkbox"/> 2229.41 lpm	<input type="checkbox"/> 1438.68 lpm	<input type="checkbox"/> 9.50 rpm	<input type="checkbox"/> 52.30	<input type="checkbox"/> 0.00
<input type="checkbox"/> 112.87 degC	<input type="checkbox"/> 128.60 degC	<input type="checkbox"/> 130.69 degC	<input type="checkbox"/> 146.20 degC	<input type="checkbox"/> 3232.00 lpm	<input type="checkbox"/> 1465.87 lpm	<input type="checkbox"/> 9.50 rpm	<input type="checkbox"/> 52.30	<input type="checkbox"/> 0.00
<input type="checkbox"/> 113.36 degC	<input type="checkbox"/> 128.47 degC	<input type="checkbox"/> 132.11 degC	<input type="checkbox"/> 147.16 degC	<input type="checkbox"/> 5234.40 lpm	<input type="checkbox"/> 1462.92 lpm	<input type="checkbox"/> 9.50 rpm	<input type="checkbox"/> 52.30	<input type="checkbox"/> 0.00
<input type="checkbox"/> 113.06 degC	<input type="checkbox"/> 132.04 degC	<input type="checkbox"/> 127.39 degC	<input type="checkbox"/> 147.51 degC	<input type="checkbox"/> 3160.71 lpm	<input type="checkbox"/> 1439.96 lpm	<input type="checkbox"/> 9.50 rpm	<input type="checkbox"/> 52.30	<input type="checkbox"/> 0.00
<input type="checkbox"/> 113.23 degC	<input type="checkbox"/> 156.75 degC	<input type="checkbox"/> 131.89 degC	<input type="checkbox"/> 148.46 degC	<input type="checkbox"/> 3070.26 lpm	<input type="checkbox"/> 1439.07 lpm	<input type="checkbox"/> 9.50 rpm	<input type="checkbox"/> 52.30	<input type="checkbox"/> 0.00
<input type="checkbox"/> 113.67 degC	<input type="checkbox"/> 158.07 degC	<input type="checkbox"/> 133.27 degC	<input type="checkbox"/> 148.69 degC	<input type="checkbox"/> 2943.86 lpm	<input type="checkbox"/> 1439.41 lpm	<input type="checkbox"/> 9.50 rpm	<input type="checkbox"/> 52.30	<input type="checkbox"/> 56.03
<input type="checkbox"/> 112.21 degC	<input type="checkbox"/> 158.56 degC	<input type="checkbox"/> 128.74 degC	<input type="checkbox"/> 149.11 degC	<input type="checkbox"/> 2925.21 lpm	<input type="checkbox"/> 1422.71 lpm	<input type="checkbox"/> 9.46 rpm	<input type="checkbox"/> 52.30	<input type="checkbox"/> 89.14
<input type="checkbox"/> 112.21 DegC	<input type="checkbox"/> 158.56 DegC	<input type="checkbox"/> 128.74 DegC	<input type="checkbox"/> 149.11 DegC	<input type="checkbox"/> 2942.94 LPM	<input type="checkbox"/> 1447.78 LPM	<input type="checkbox"/> 9.46 RPM		

POSITION	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
FACTOR	<input type="text" value="0.00"/>	<input type="text" value="0.00"/>	<input type="text" value="0.00"/>	<input type="text" value="0.00"/>	<input type="text" value="0.00"/>	<input type="text" value="0.00"/>

KAPPA CORRECTED	<input type="text" value="174.14"/>
-----------------	-------------------------------------

Figure 3-7 : GUI- main interface

On the bottom right hand corner, the “Kappa corrected” gives the prediction of present Kappa number from the Smith predictor.

The third line from the bottom is where the values of the monitored parameters are displayed. These values are updated as soon as the DCS refreshes the system. They are then stored in the model. Every hour the average over a period of 60 minutes is stored. The value is then displayed in the line above. The operator can check if there is a significant change between the previous

values and the current ones. The history of the values goes up to 6 hours. Thus, it is possible to choose the specific value of the parameters we want to isolate on the model. For example, if the model requires the value of the top temperature 2 hours ago, this value is selected by clicking on the button next to the appropriate entries (Figure 3-8).

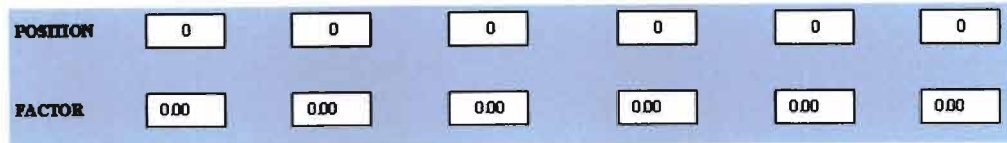


Figure 3-8: GUI- factors

3.3 The Time-Shifting process

The simple linear model obtained ignores the obvious distributed nature of the process. The data were simply lumped at one point in time for the purpose of regression. But the 8 to 12 hour journey through the digester would render this model inappropriate if the key parameters happen to be experienced at an early stage. In order to account for this, a “time-shifting” process was necessary in this case.

Clearly these shifts, once identified, need to be used to synchronise particular measurements appropriately to correspond to the chips leaving the reactor i.e. the exit point at the bottom of the digester was considered as the reference point relative to which all other plant measurements had to be synchronised. Thus, it was imperative to determine which measurements were subjected to time-shifting. The temperature measurements at the top of the digester were prime candidates to which these time-shifts could be applied.

In order to synchronise all plant measurements with respect to the exit point at the bottom of the digester, it was assumed that the residence time of the digester is approximately eight hours. The digester in question consists of 4 zones as previously mentioned. Thus it was presumed that the wood chips spend a period of two hours in each zone. Using this as a basis, time-shifts were applied with each time-shift interval representing a shift of 2 hours, in initial off-line tests.

The process of time-shifting a selected measurement is best explained with the aid of an example. Consider the liquor phase temperature located at the top section of the digester i.e. at the impregnation zone (Figure 4-1, zone I). To synchronise this measurement with the exit point of the digester, it was required to look eight hours further back in time (Figure 3-9). In the off-

line data analyses, this could be accomplished by shifting the spreadsheet column of data of the selected measurement by four intervals of two hours each when considering the fact that measurements of basic process variables were logged at two hourly intervals. Similarly, any measurement located in the first cooking zone (Figure 4-1, zone II) would have to be shifted by three intervals and so on.

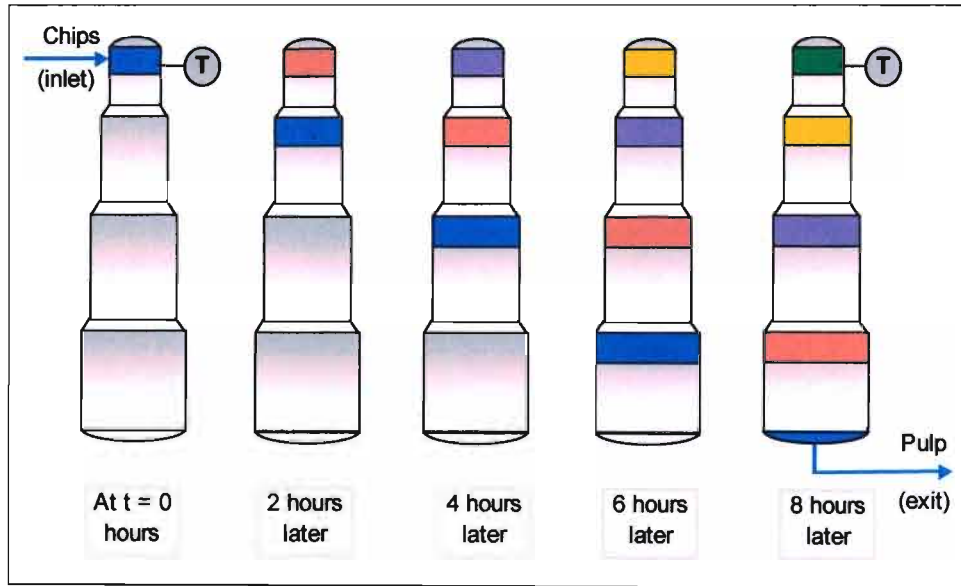


Figure 3-9: Illustrating the distributed nature of the Kraft process

Various time shift combinations were then applied to the selected measurements, and each time a new model was regressed using the shifted data set. With each “time-shift combination” applied, the standard deviation between the measured Kappa and the predicted Kappa number was computed. The standard deviation was computed with the aid of the following statistical formula:

$$\text{Standard deviation} = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (k_i - k_m)^2} \quad (3.1)$$

where N = Number of data points

k_i = Predicted Kappa number

k_m = Measured Kappa number

The best shift combination was then determined as that minimising the standard deviation of the model error.

CHAPTER 4

Off-line and On-line Tests

After considering the digester and its numerous parameters, the variables listed in Table 4-1 have been chosen as having the most significant effect on the final Kappa number. These measurements may be located in Figure 4-1. A short description and the identification tag is given in each case in the table.

#	Description	Tag Id.
1	Top Circ Temp	TI 3012
2	Dig. Phase Temp	TI 3126
3	Circ Temp Before C8	TI 3108
4	Temp Adj Before C6	TI 3100
5	Upper Circ Flow	FFIC 3105
6	Bottom Circ Flow	FFIC 3112
7	Chip Moisture	-

Table 4-1: Key parameters chosen for the model.

As presented in Chapter 3, the processing of the data involves a time-shifting step. We will present in Section 4-1 the results obtained without any time-shifting and will apply it to the set of data in the Section 4-2.

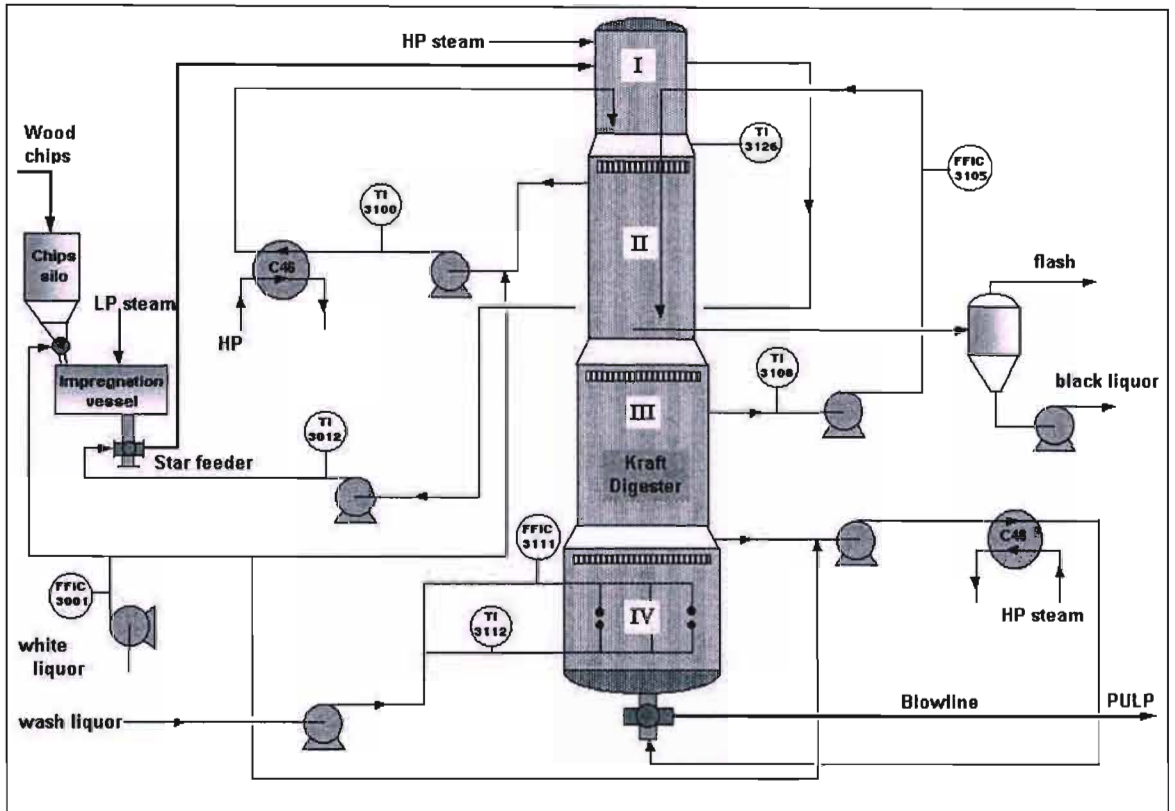


Figure 4-1: Representing the process flow diagram of the Kraft digester
(adapted from Jagarnath & Joseph, 2004)

Depicted in Figure 4-1 are the different zones of a Kraft digester

- Zone I: impregnation zone
- Zone II: cooking zone (co-current stream)
- Zone III: cooking zone (co-current stream)
- Zone IV: washing zone (counter-current zone)

4.1 Unshifted set of data

The model being a first-order linear regression, it requires seven coefficients, plus an eighth parameter for the *bias*. This commonly expressed as $y = \sum a_i x_i + b$, where the a_i and b are constants. The unshifted set of data processed through the linear regression gave the parameters listed in Table 4-2.

No.	Parameter	Tag No.	Coefficients
1	Top Circ Temp	TI 3012	0,0355254
2	Dig Phase Temp	TI 3126	0,1687534
3	Circ Temp Before C8	TI 3108	-0,11496874
4	Temp Adj Before C6	TI 3100	-0,20958635
5	Upper Circ Flow	FFIC 3105	0,00097889
6	Wash Dig Nozzle	FFIC 3112	0,00106983
7	Chip moisture content	-	-0,53463345
8	BIAS	-	87,0827858
Model: R-squared = 0.104			

Table 4-2: Representation of the key parameters and the coefficients

In order to get an idea on how the model will react to new data, i.e. data not used in the original regression, the coefficients will be applied to the regression data (“seen”), as well as a new period of plant data (“unseen”) for comparison of the quality of Kappa number prediction.

Figure 4-2 represents predictions using one of the first sets of coefficients obtained by regression. As noted above, the “unseen” set means that the model is given new values of the digester measurements in a period other than that used for regression.

The results obtained (Figure 4-2) are not satisfactory: although the pattern of the Predicted Kappa follows the Measured Kappa, there is still some delay in the “seen” part. The model performance in the “unseen” part is poor, and shows a certain lack of flexibility of the model.

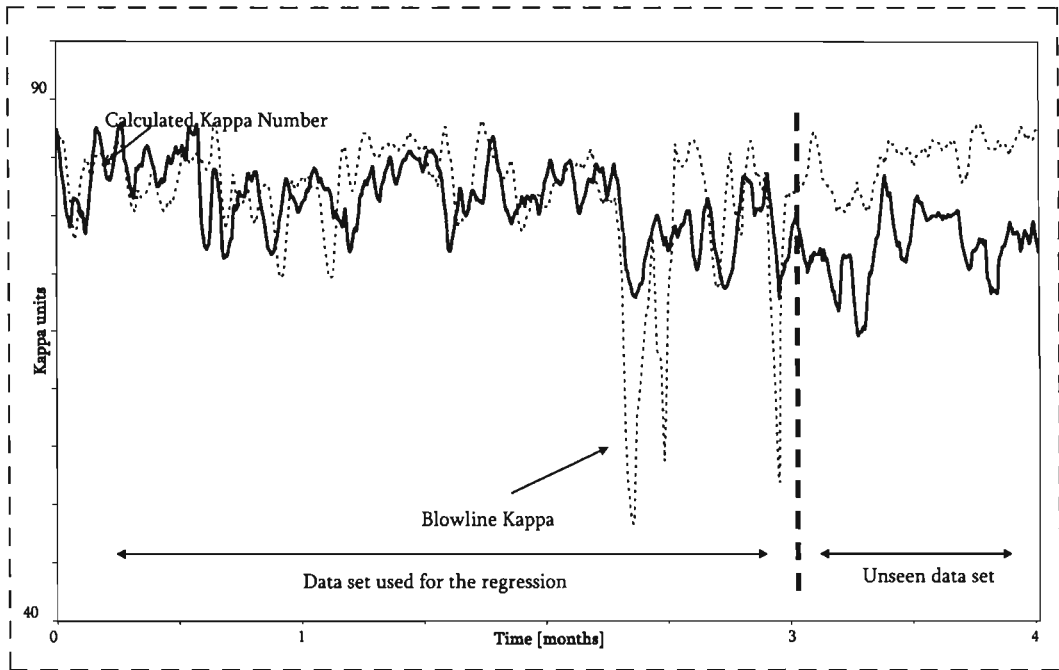


Figure 4-2: Variation of the measured Kappa number and the predicted Kappa number with time on a seen and an unseen set of data

4.2 Time Shifting

As stated previously, the time shifting process is needed to phase predictions of the final Kappa number with the conditions experienced during plug-flow through the reactor. Various combinations of time-shifts were applied to certain selected key process variables.

A time-shift represented as a value of one unit equals to a period of two hours. Hence, in Table 4-3, “1” represents a shifting, to an earlier time, equivalent to a period of two hours, “2” equals a shift to four hours earlier, etc.

Combination Number	Number of Time-Shifts				Standard Deviation	Model R-Squared
	TI 3126	TI 3100	TI 3012	FFIC 3105		
1	0	0	0	0	7.359978	0.230
2	1	1	1	1	7.300253	0.233
3	2	2	2	1	7.282239	0.235
4	3	2	3	1	7.279223	0.238
5	1	1	1	0	7.310082	0.233
6	2	2	2	0	7.316531	0.235
7	3	2	3	0	7.292452	0.236
8	1	0	0	0	7.329885	0.226
9	1	1	0	0	7.357673	0.226
10	2	1	0	0	7.324871	0.231
11	2	2	0	0	7.251734	0.239
12	2	1	1	0	7.263517	0.238
13	2	1	2	0	7.276533	0.237

Table 4-3: Representing the standard deviation between the predicted Kappa number and measured Kappa number for each time-shift combination applied

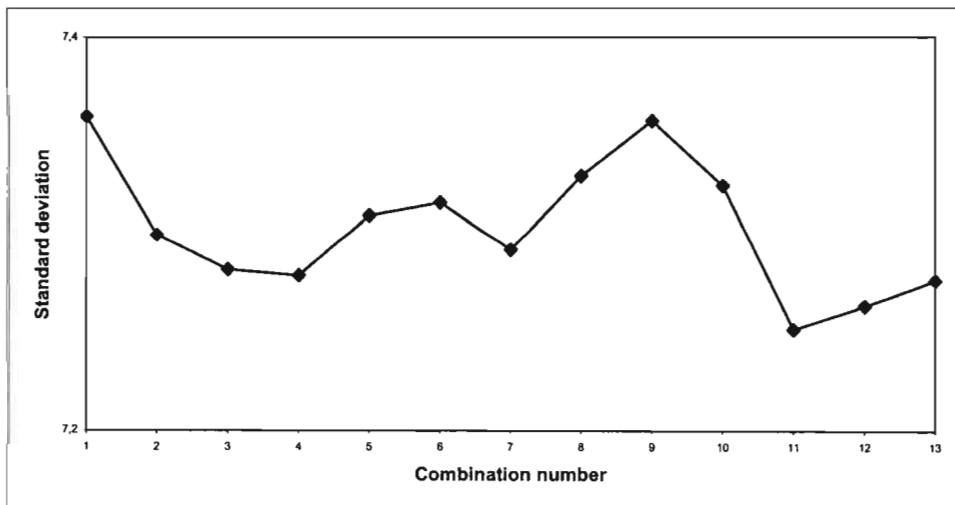


Figure 4-3: Standard deviation for each time-shift combination

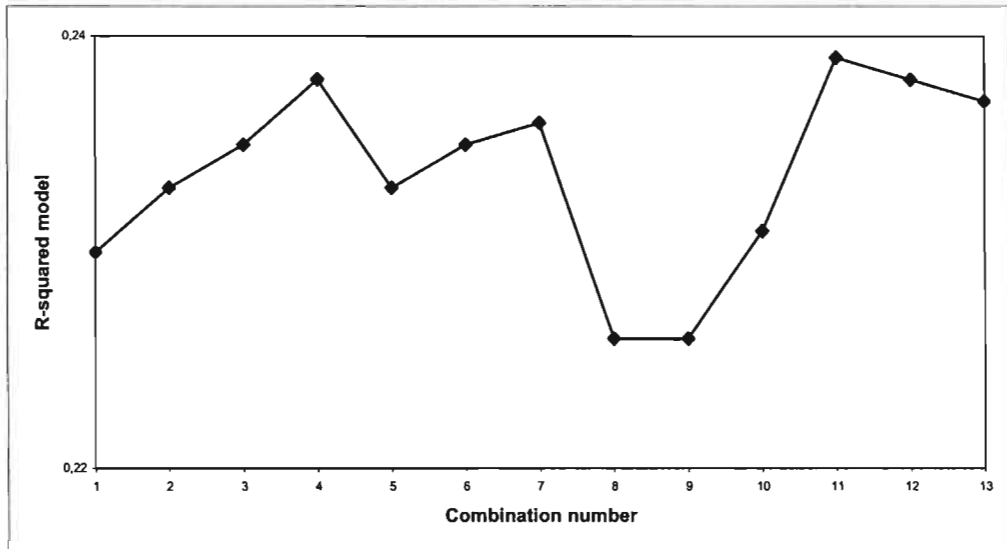


Figure 4-4. R-squared model for each time-shift combination

Based on the Figures 4-3 and 4-4, it can be seen that the eleventh combination is the optimum combination: it has the smallest standard deviation and highest R-squared value. Therefore, in order to synchronise all plant measurements, the fixed time-shift positions in Table 4-4 should be applied to the relevant measurements:

Measurement	Tag Id.	No. of time-shifts	Fixed Position
Dig Phase Temp	TI 3126	2	- 4 hours
Temp Adj Before C6	TI 3100	2	-4 hours

Table 4-4: Representing the fixed time-shift positions

The concept of the “fixed position” may be explained as follows:

Consider obtaining a model prediction for Kappa number at the reactor exit at time t . Plant measurements for the ‘Dig Phase Temp’ and ‘Temp Adj Before C6’ should both be accessed 4 hours prior to time t , to achieve synchronisation with the remaining measurements.

Re-regressing the data set with these shifts, the regression coefficients listed in Table 4-5 were established.

No.	Parameter	Tag No.	Coefficients
1	Top Circ Temp	TI 3012	0,0360014
2	Dig Phase Temp	TI 3126	0,18609284
3	Circ Temp Before C8	TI 3108	-0,11565567
4	Temp Adj Before C6	TI 3100	-0,19123035
5	Upper Circ Flow	FFIC 3105	0,00072027
6	Wash Dig Nozzle	FFIC 3112	0,00122623
7	Chip moisture content	-	-0,58254456
8	BIAS	-	113,882866
Model: R-squared = 0.185			

Table 4-5: Representing the regression coefficients for the eight selected parameters as well as the model R-square value where the optimum time shift combination had been applied to the data set

Thus the final model for the ‘Kappa-Predictor’ can be represented by the following equation (Table 4-6).

$ \begin{aligned} \text{Kappa} &= 0,0360014 * (\text{Top Circ Temp}) \\ &+ 0,18609284 * (\text{Dig Phase Temp}) \\ &- 0,11565567 * (\text{Circ Temp Before C8}) \\ &- 0,19123035 * (\text{Temp Adj Before C6}) \\ &+ 0,00072027 * (\text{Upper Circ Flow}) \\ &+ 0,00122623 * (\text{Wash Dig Nozzle}) \\ &- 0,58254456 * (\text{Chip Moisture}) \\ &+ 113,882866 \end{aligned} $
--

Table 4-6: Regressing coefficients

This model is based on the following fixed positions:

Measurement	Fixed time-shift position
Dig Phase Temp	-4 hours
Temp Adj Before C6	-4 hours

Applying the model from Table 4-5, to the regression and unseen data sets, the Figure 4-5 was obtained:

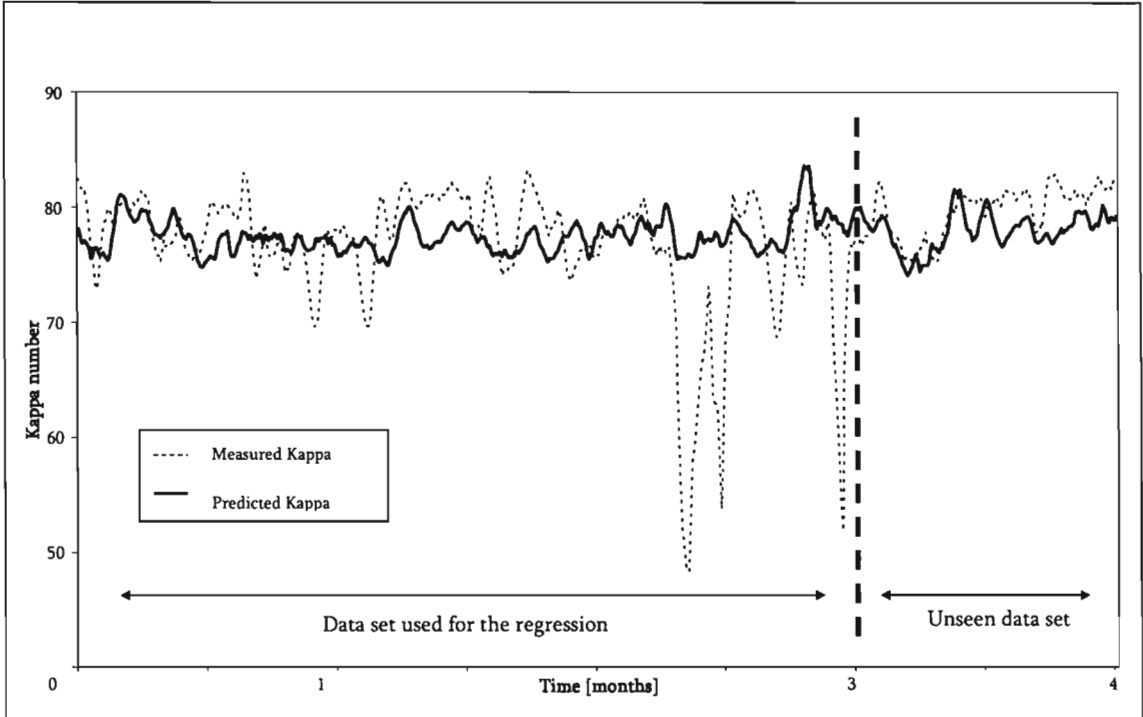


Figure 4-5: Depicting the variation of the measured Kappa number and the predicted Kappa number with time (Optimum time shift combination)

We can already see an improvement in Figure 4-5: the unseen data set is better fitted by the model with less error amplitude. These results are discussed further below.

4.3 Discussion

As stated, the major objective of this study was to develop a model that would provide the means to predict the Kappa number of the product pulp in real time for a continuous Kraft digester located at the SAPPI-Tugela Paper Mill. The aim was to allow corrective actions to be undertaken earlier than allowed by the intermittent laboratory analysis of the Kappa number (usually every two hours). It was proposed to develop a model for this, possibly allowing operation under closed-loop control.

Parameters to be incorporated in the model initially consisted of plant data based on the following:

- Temperature measurements
- Bottom circulation flow
- Upper circulation flow
- Chip moisture content

These parameters were chosen amongst many others based on their importance in the digester. It is obvious that other essential parameters could have been incorporated. We can list some of them that could have a significant impact on the Kappa number prediction:

- Wood species
- Density
- Chip dimensions
- Chemical components of the cooking liquor
- The concentration of the cooking chemicals

Some parameters were not recorded at the beginning of the study and others, like the wood species, are still not identified on the mill.

Where possible, these parameters should be incorporated. Indeed, considering hardwoods and softwoods, the rate of delignification is considerably faster in hardwoods than in softwoods. As for the density, it is clear that the impregnation will be different bearing in mind the fact that dense woods are more difficult to impregnate. This would result in a higher Kappa number. In the same way, the chip size is important during the pre-cooking process. Indeed, a thicker chip will be harder to cook entirely, possibly leaving its heart undercooked. On the contrary, a thin chip could be overcooked. The Kappa number will be affected anyway. The different chemical agents used (white, black, green liquors) and their concentrations are also important. They are fundamental to the process and have a direct impact on the digestion. It is obvious that this information should be incorporated.

Despite omitting these parameters, the model was believed adequate to reflect the process and to obtain a useful Kappa number estimate. A linear regression with the inclusion of a bias was applied to plant measurements chosen between December 2001 and December 2003. Although

the system displays complex non-linear behaviour, a linear model was selected for simplicity. It is a simple yet effective model.

As stated previously, two sets of data were used. The first one, the “seen” set, was for the regression part in order to obtain the coefficients of the model and the second one, the “unseen” set, was used to test the model and its validity and also to analyse the model’s behaviour when confronted with unexpected situations.

The initial model obtained from a simple linear regression did not take into consideration the distributed nature of the process. This arises from the long residence times experienced in the digester. In order to account for this, all measurements were required to be synchronized relative to a reference point, in this case, the exit point at the bottom of the digester. This entailed the application of the time-shifting procedure, which has already been discussed.

Looking at figures 4-3 and 4-4, it is noticeable that the standard deviation between the predicted and measured Kappa numbers and the model R-squared value is inversely related. The optimum time-shift combination was selected on this basis i.e. the combination that resulted in the smallest standard deviation and the largest R-squared value was considered to be the optimum time-shift. The shifts obtained were acceptable, however they did not exactly agree with what was expected based on the sensor locations. This could be attributed to the variations in the residence times (i.e. 8-12 hrs) experienced in the digester as process flow changes.

Figures 4-2 and 4-5 depict the results obtained before and after the time shifting. There is an obvious lack of precision in figure 4-2 regarding the unseen data set. Figure 4-5, where the time shift is operated, reveals a satisfactory pattern of the model in the seen data set and a rather good adaptation to the unseen data set. The time shifting turns out to be responsible for this improvement in the modelling and confirms the importance of the time-delay resulting from the long digester residence time.

Despite the above, the improvement the final correlation obtained (from 0.104 to 0.185) shows clearly a poor fit from a mathematical point of view. In spite of this, the model was implemented on the site as it gives nevertheless acceptable results on the Kappa number prediction. The low significance of the regression could be explained by a poor choice of parameters for the model. The poor correlation may also result from the crude time-resolution of collected data, or from the possibility that not all important influencing variables were available as continuous measurements. Furthermore, there may be significant non-linearity in the true relationships.

These results may explain why a simple linear regression has never been explored before. Indeed more complex ways were studied in order to get as close as possible to the reality.

A recent study (Jagarnath and Joseph, 2004), including more parameters and possibly confirming another approach should be investigated, shows that some of the parameters originally chosen may not have been the best choices. Indeed, it can be seen that the circulation temperature before C8 (Tag no. TI 3108) should be eliminated as it yielded the smallest absolute value of both the Zero-Order and Partial correlation coefficients suggesting that it is a weak predictor of the Kappa number (Appendix C). It is important to note that the original on-line module with seven plant measurements from the digester had to be used. Thus, Jagarnath and Joseph (2004) had to remove two parameters from their selected nine parameters, to fit it into the existing on-line module. Figure 4-6 shows the quality of their regressed model.

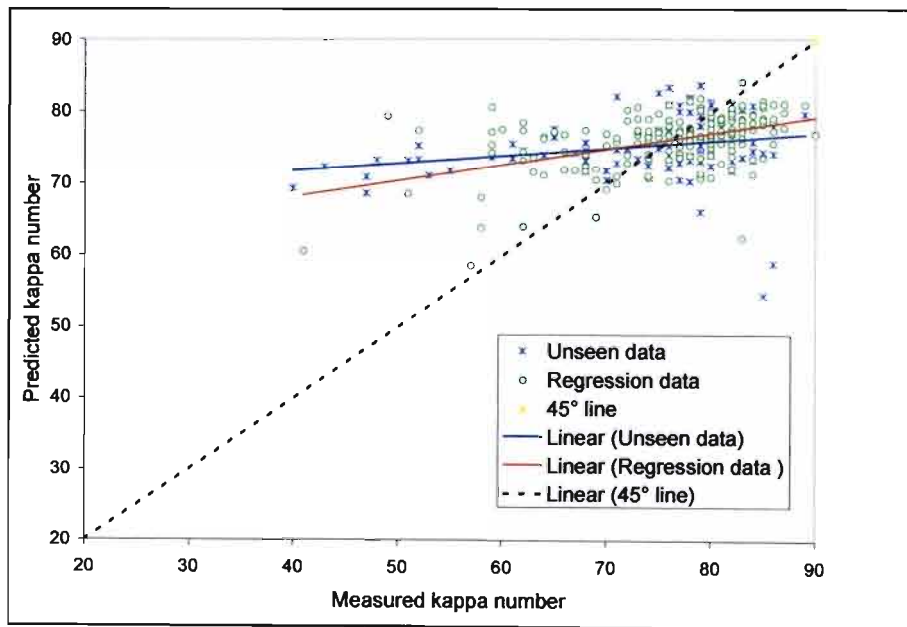


Figure 4-6: Final model predictions vs. measured Kappa number for both the regression and unseen data sets (Jagarnath and Joseph, 2004)

Upon attaining the final “Kappa-Predictor” model based on the eight parameters with the fixed time shift positions applied, Figure 4-6 was obtained which depicted the measured against predicted Kappa number for all data points from both the regression data set as well as the unseen data set. The fitted lines show similar behaviour of the predictions for seen and unseen data, viz. over-prediction at lower Kappa numbers.

Possible sources of model error include:

- Important parameters such as the chip size and wood type were not incorporated in the model.
- Variations in digester residence time: 8-12 hours
- Variations in laboratory measurement delay: time delay from sampling to measurement availability not necessarily fixed at two hours as assumed.

At SAPPI-Tugela, the measurements of the basic process variables are continuously available, but important pulp characteristics such as the Kappa number are only available from intermittent (every 2 hours) laboratory analysis. Samples of the product pulp are taken in order to measure the Kappa number and a measurement of the Kappa number is only available approximately two hours later. Hence, there would be a time delay between the measured Kappa number and the predicted Kappa number should the “Kappa-Predictor” model be implemented on the plant. The on-line system deals with this by delaying predictions by a fixed 2-hours before comparison with a new laboratory analysis.

4.4 Smith Predictor

To compensate for the laboratory measurement time delay (or dead-time) requires the application of the Smith Predictor. When applied for the control of the Kraft digester, it is responsible for comparing the laboratory analysis of the Kappa number with a delayed synchronous predicted value, implying that old errors will be used to correct the current model predictions. The Figure 4-7 is a scheme based on the Smith Predictor model with possible closed-loop control.

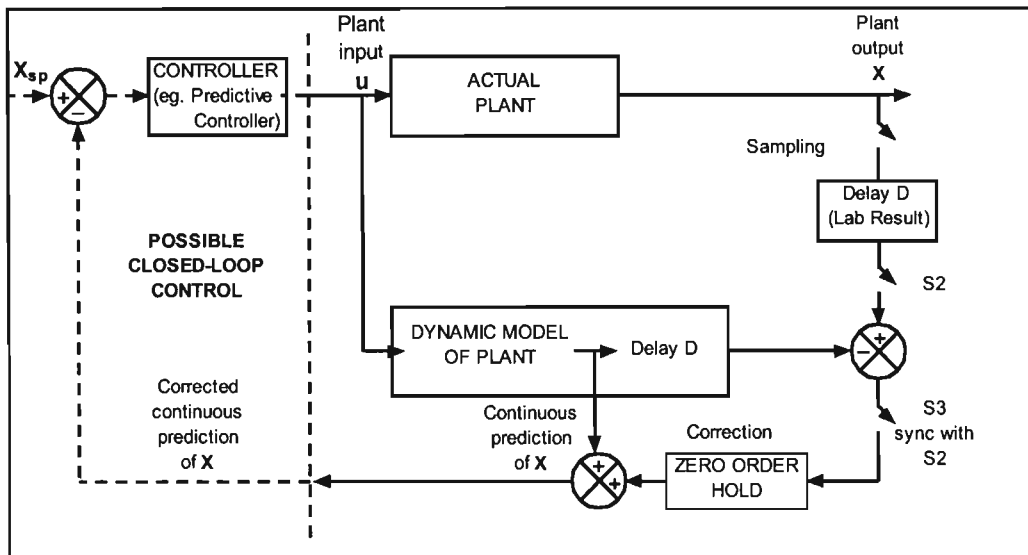


Figure 4-7: Scheme for the prediction of the Kappa number with intermittent correction synchronised by a Smith Predictor (Mulholland, 2002)

The interesting feature of the Smith Predictor, as depicted in figure 4-7, is that the model predictions of the Kappa number are delayed i.e. they are continuously held in a “stack”. When a laboratory measurement of the Kappa number becomes available, it is compared with the appropriate prediction by searching back through the stack. The correction computed is held and is continuously used to correct the current model predictions until a new laboratory measurement becomes available to allow for the computation of a new correction.

Code written in MATLAB has been developed for the off-line testing of the “Kappa-Predictor” model based on the Smith Predictor, using the plant data available. The selected plant measurements on which the model is based are held in a local stack within the program stretching back 20 hours. The fixed positions obtained from the time-shifting procedure are used in order to locate the appropriate point that each measurement should be accessed. These positions are used to look backward in time for certain measurements to achieve synchronisation among all the key measurements for prediction purposes. In this way, the measurements are lumped at the exit point of the digester, and are used to predict the Kappa number at that instant. However, due to the intermittent laboratory analysis of the product pulp (usually every two hours), there is a further delay of 1-2 hours before the laboratory is able to provide the appropriate Kappa measurement. Therefore, the local stack also stores raw uncorrected model predictions for “lookup” according to the sample ‘time-stamp’ to ensure that an appropriate correction can be applied in the Smith Predictor. It should also be noted that some smoothing is applied to the model correction to

account for “more average” offset errors and not “bump” predictions too much in the event of incorrect phasing.

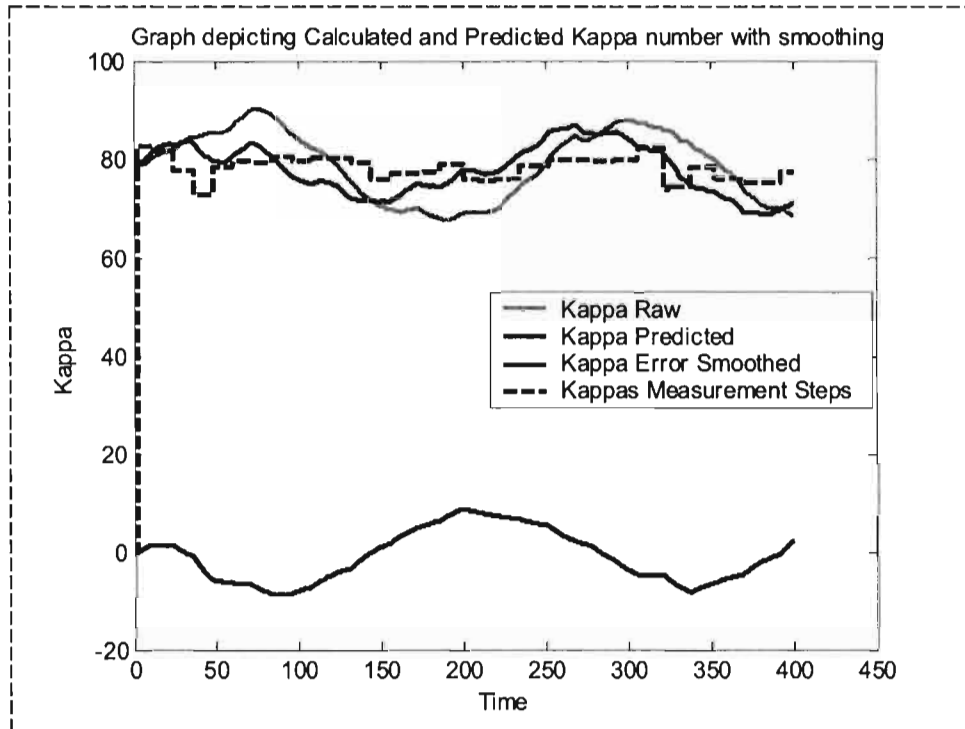


Figure 4-8: Real-time model predictions vs. measured Kappa number for the period on which the regression data was based. These predictions include time shift compensation as well as smoothed error correction

The curves represented in figure 4-8, an off-line MATLAB simulation using actual plant data, illustrate the following:

- **Kappa raw** is the raw prediction obtained from the plant model.
- **Kappa meas. Steps** represents the laboratory measurements of the Kappa number at random times (actual measurement point is at the start of each step)
- **Kappa error smoothed** is the error or correction obtained from a comparison of the measured Kappa number with the appropriate predicted Kappa number. As previously mentioned, some smoothing was applied to the corrections.
- **Kappa predicted** is the outcome of applying the smoothed correction to the raw Kappa prediction.

CHAPTER 5

Conclusions and Recommendations

This chapter comprises two parts. Firstly the conclusion summarizes, in point form, the main findings from this research study. Thereafter the recommendation section suggests areas of further concern regarding this work and possible methods of solution.

5.1 Conclusion

1. A model for the prediction of the blowline Kappa number was developed based on seven process variables. The two major challenging characteristics noted during this study were the long residence times experienced in the digester and the fact that the Kappa number was only measured intermittently, with a delay before it became available. The long residence times would have had an adverse impact on the model, resulting in unsynchronized plant measurements. However, this was overcome by a procedure of “time-shifting”. To deal with the laboratory measurement delay, raw predictions were also delayed until the appropriate laboratory result was input manually, in order to compute a correction term.
2. Code was developed for the implementation of this model on-line at SAPPI-Tugela whereby the model predictions are corrected intermittently. These intermittent corrections, synchronized by the Smith Predictor, were embodied within the developed code.
3. The model has been incorporated into the plant DCS. Future work entails the analysis of the captured process data from the plant which would provide the means to make adjustments to the model and thus improve model predictions.
4. The ultimate objective is to produce a model that is capable of managing the process with as little intervention from the plant operator as possible ie. to allow the plant to operate under closed-loop control.

5.2 Recommendations

1. The regressed model of the process, showing the dependence on key measurements, could form the basis of a closed-loop Kappa number controller, by optimal simultaneous manipulation of several variables on the plant. Feedback would of course be provided by this observer model for Kappa number.
2. The simplicity of the proposed model gives it robustness. However, further operational data should be collected for future updating of the proposed model, including additional plant variables.
3. This model presents a “black box” view of the digester. Interpretation of the chemical reactions taking place in the digester could be another way of modelling a Kraft digester.
4. The laboratory results are taken every two hours. Although the Kappa number should not vary very quickly, this sampling period should be reduced in case of any unusual occurrences, i.e. major Kappa deviation.

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Appendix A

Matlab codes

A.1 DCSprog.m

```
% DCS Program to predict Kappa number with asynchronous Smith
Prediction

% Initialisation

clear all;
TRUE = 1;
FALSE = 0;

% Time structure

t=0; % Absolute time at start-up
(need to initialise to clock) [hours]
tend = 400; % Normally infinity [hours]
dt=0.1; % Cycle time of this algorithm
as strobed by the DCS [hours]
npt=tend/dt+1 % number of plot points allowed
for
P_KappaNowPredicted = zeros(npt,1); % plotting array
P_KappaRaw = zeros(npt,1); % plotting array
P_KappaMeasSteps = zeros(npt,1); % plotting array
P_KappaErrorSmooth = zeros(npt,1); % plotting array
P_t = zeros(npt,1); % plotting array
KappaMeasSteps=0; % for plotting
nP = 0; % initialise number of plot
points

% Buffer file
nBuffer = 200; % Length of buffer file spaced
at dt : need 20 hours max
nmeas = 7; % Number of plant measurements
Buffer = zeros(nBuffer,nmeas); % Cyclic buffer file
pBuffer = nBuffer; % Buffer file pointer position
firstcall =1; % flag to warn of firstcall

% Laboratory Buffer
nLabBuf = 400; % Length of buffer file spaced at
dt : could need to go back a long way
LabBuf = zeros(nLabBuf,1); % Cyclic buffer file
pLabBuf = nLabBuf % Lab buffer file pointer
position
```

Appendix A: Matlab codes

```
% Kappa Error smoothing filter
alpha=0.005; % Need to calculate this in
terms of dt ##### done on every dt step !
KappaError = 0; % Leave at zero until first
calculated
KappaErrorSmooth = 0; % Initialise to zero

% mass-volumes back to points of measurement
mv = zeros(1,nmeas);
mv(1)=6*2700; % only relevant before re-calibration
mv(2)=0; % #### need to put plant figures in here !
mv(3)=0;
mv(4)=0;
mv(5)=0;
mv(6)=0; % for this example the first reading is assumed to
be flow in [mv / hour]
mv(7)=0;

% default values in case of measurement failure at the start-up
% (else it takes the last valid measurement)
last_valid_meas_synchronised(1) = 110.67; % #### realistic
figures required here
last_valid_meas_synchronised(1) = 136.5;
last_valid_meas_synchronised(1) = 130.83;
last_valid_meas_synchronised(1) = 137;
last_valid_meas_synchronised(1) = 2833.5;
last_valid_meas_synchronised(1) = 4695;
last_valid_meas_synchronised(1) = 54.5;

while t<=tend
    t=t+dt;
    pBuffer = pBuffer+1;
    if (pBuffer>nBuffer)
        pBuffer = 1; % Wrap it back
    end
    meas=readplant(t); % Read data from the plant I/O
interface

    if ~firstcall
        Buffer(pBuffer,:)=meas; % overwrite oldest entry
    else
        for i=1:nBuffer
            Buffer(i,:)= meas; % initialise the buffer file at
the start
        end
    end

    % Integrate the flow (measurement 1) backwards until you hit the
% desired mass-volume
    Bin = zeros(1,nmeas);
    mvint= zeros(1,nmeas);
    for i=1:nBuffer
        Bp = pBuffer-i+1;
        if (Bp<1)
            Bp=Bp+nBuffer; % Wrap it back
        end
    end
end
```

Appendix A: Matlab codes

```
end
for j=1:nmeas
    if (mvint(j)<=mv(j))
        mvint(j) = mvint(j) + Buffer(Bp,5)*dt; % assumes
that the wood-chip flow is in meas position 5####
        Bin(j)=Bp; % this is also protection for very low
flows : will set to last available
    end
end
end

%y=      -0.278752479      * TR 4-6 + 0.23785753 *TR 41-8 + -
0.281104622      *TR 8-1+  0.824952165      *TR 6-2      0.002419298
      *FI 7-3 +  0.006031395      *FRC 9-1+  -0.199681051      * CM +
      -19.9652196

% Regressed coefficients for present conditions:
coeff = zeros(7,1);

coeff(1)=-0.278752479;
coeff(2)=0.23785753;
coeff(3)=-0.281104622;
coeff(4)=0.824952165;
coeff(5)=0.002419298;
coeff(6)=0.006031395;
coeff(7)=-0.199681051;
bias = -19.9652196;

% Predict the Kappa number with the delayed data
meas_synchronised = zeros(1,nmeas);
for j=1:nmeas
    meas_synchronised(j)=Buffer(Bin(j),j);
    if(meas_synchronised(j)>=0)
        last_valid_meas_synchronised(j)=meas_synchronised(j); %
protect against faulty data
    else
        meas_synchronised(j)=last_valid_meas_synchronised(j);
    end
end
KappaRaw = meas_synchronised*coeff + bias; % scalar value

% includes error for testing purposes
% *****Take out in the plant
*****
errorfreq=0.1;
erroramp=10;
error=erroramp*sin(errorfreq*2*3.1415*t/24);
KappaRaw=KappaRaw+error;
% *****Take out in the plant
*****

% write raw prediction to Lab buffer file
pLabBuf = pLabBuf + 1; % increment predictions file pointer
if (pLabBuf > nLabBuf)
    pLabBuf = 1;
```

Appendix A: Matlab codes

```
end
if ~firstcall
    LabBuf(pLabBuf)=KappaRaw;    % overwrite oldest entry
else
    for i=1:nLabBuf
        LabBuf(i)= KappaRaw;    % initialise the buffer file at
the start : will lead to some inaccuracy at start
    end
    firstcall=FALSE;           % reset the firstcall flag now
end

% See if a laboratory analysis has become available
kappasample = checklaboratory(t,dt);
KappaSampleTime = kappasample(1);
KappaSampleMeas = kappasample(2);
if (KappaSampleTime >= 0)
    % A sample has just become available in this interval
    tsample = KappaSampleTime;
    tgap= min(0,t-tsample);    % can't be in the future !
    intgap = floor((tgap/dt) + 0.5);
    iLabBuf = pLabBuf - intgap;
    if (iLabBuf < 1)
        iLabBuf = iLabBuf + nLabBuf;    % wrap it back
    end
    %..... so.... what prediction was synchronous at that time
    KappaRawThen = LabBuf(iLabBuf);
    KappaError = KappaSampleMeas - KappaRawThen;
    KappaMeasSteps = KappaSampleMeas;
end

% Finally we get the present prediction with Smith correction
KappaErrorSmooth = alpha * KappaError + (1-
alpha)*KappaErrorSmooth;
KappaNowPredicted = KappaRaw + KappaErrorSmooth;

nP = nP + 1;
P_KappaNowPredicted(nP) = KappaNowPredicted;
P_KappaRaw(nP) = KappaRaw;
P_KappaErrorSmooth(nP) = KappaErrorSmooth;
P_KappaMeasSteps(nP) = KappaMeasSteps;
% (#### Could use above arrays for standard deviation calculation
% with different "mass-volumes" : KappaRaw vs
KappaSampleMeas(full set) )
P_t(nP) = t;
end

% Plot results

plot(P_t(1:nP),P_KappaRaw(1:nP),'g',
P_t(1:nP),P_KappaNowPredicted(1:nP),'r',...
P_t(1:nP),P_KappaErrorSmooth(1:nP),'b',
P_t(1:nP),P_KappaMeasSteps(1:nP),'y');
title('Graph depicting Calculated and Predicted Kappa number with
smoothing')
xlabel('Time');
ylabel('Kappa');
```

Appendix A: Matlab codes

```
legend('Kappa Raw', 'Kappa Predicted', 'Kappa Error  
Smoothed', 'Kappas Measurement Steps');
```


A.2 Interpolate.m

```
% SAPPI Data Processing

SetA;

nsmooth=9; % use odd for centred smooth

[n m]=size(A);
B=A;
B(1,:)=A(1,:);
for j=1:m
    ilast=1;
    for i=2:n
        if A(i,j)~=0
            B(i,j)=A(i,j);
            if ilast==i-1
                ilast=i;
            else
                for ii=(ilast+1):(i-1)
                    B(ii,j)=((ii-ilast)/(i-ilast))*(A(i,j)-
A(ilast,j))+A(ilast,j); % linear interpolation
                end
            end
            ilast=i;
        end
    end
end

nsmooth=11; % use odd for centred smooth
C=B;
for i=1:n
    acc=0*B(i,:);
    is=max(1,i-floor((nsmooth-1)/2));
    ie=min(n,i+floor((nsmooth-1)/2));
    for ii=is:ie
        acc=acc+B(ii,:);
    end
    C(i,:)=acc/(ie-is+1);
end

fC=fopen('C.txt','w');
for i=1:n
    for j=1:m
        fprintf(fC,'%9.2f',C(i,j));
    end
    fprintf(fC,'\n');
end
fclose(fC);
```

A.3 Readplant.m

```

function measurement = readplant(time)
%Time - T4-6 - T41-8 - T8-1      - T6-2      - F7-3      - F9-1 - CM
% Get Plant Measurements at this (present) time
% Measurement array: 1st column is some time measurement
Data = [0 110.7 136.5 130.8 137.0 2833.5      4695.0      54.5
2      110.9 136.4 131.1 136.9 2834.4      4710.0      54.2
4      111.0 136.6 132.0 137.4 2742.6      4546.3      54.2
6      111.1 136.0 132.6 137.9 2669.0      4458.9      54.3

3010 112.0 140.6 121.1 135.4 5119.0      1595.8      45.3
3012 112.0 140.2 120.9 135.3 5119.0      1611.1      44.2
3014 112.1 140.1 120.3 135.3 5119.0      1636.1      42.9
3016 112.1 140.1 119.5 135.4 5119.0      1634.6      41.2
3018 112.3 140.1 119.0 135.6 5119.0      1634.3      39.4
3020 112.7 140.2 119.0 135.7 5119.0      1635.8      37.4

];

tdat = -999;
idat = 1;
while tdat < time          % find a file time just greater than
"time"
    idat=idat+1;
    if idat > size(Data,1)
        idat=size(Data,1);
        break;
    end;
    tdat=Data(idat);
end
idats = idat-1;
idate = idat;
tgap = Data(idate,1)-Data(idats,1);
fract = min(max(0, (time-Data(idats,1))/tgap),1);    % fraction of
way across the gap

nmeas = size(Data,2)-1;
measurement = zeros(1,nmeas);
for i=1:nmeas
    if ((Data(idats,i+1)>0) & (Data(idate,i+1)>0)) % both ends valid
        measurement(i)=(1-fract)*Data(idats,i+1) +
(fract)*Data(idate,i+1);    % linear interpolation
    else
        measurement(i)=-999;    % there are faulty measurements
    end
end
present
end
end

```

A.4 SetA.m

```
% Sets up data input for "Interpolate"
A=[111      135  127  139  2825  4577  7.5  56.5  83
111  138  129  136  2831  4525  7.5  0  82
109  140  132  141  2840  4708  7.6  54.6  80
111  132  131  134  2820  4820  7.6  0  83
111  137  132  137  2825  4740  7.5  53.4  84

114  147.1  125.9  147  2435  1501  0  0  74
111  145  133  146  2500  2063  0  52.9  84
0  0  0  0  0  0  0  0  85
112  157  131  149  2680  2036  0  53.7  85
113  152  133  145  2650  1621  0  0  83
113  150  135  146  2850  1589  0  55.9  87
113  153  131  148  0  1707  0  0  80
113  144  146  144  2450  1217  0  0  60
112  146  145  143  0  1220  0  53.9  62];
```

A.5 Checklaboratory.m

```
function kappasample = checklaboratory(time,dt)

% Check if a new Kappa measurement is available :
% [available time, sample time, lab measurement]
% Note: these will be asynchronous & randomly spaced

% ##### must delete rows randomly below !!!
KappaData = [2  0  82.5
12  10  81.7
24  22  77.6

2918  2916  76.4
3012  3010  73.8
3020  3018  69.9
];

kappasample = [-999 -999]; % No sample has appeared
ts=time-0.5*dt;
te=time+0.5*dt;
tdat = -999;
idat = 0;
while ((tdat<=ts)|(tdat>te)) % find a file time just greater
than "time"
    idat=idat+1;
    if idat>size(KappaData,1)
        return;
    end;
    tdat=KappaData(idat,1);
end

% A new analysis is available
KappaData(idat,1)=-tdat; % show that this has been seen & acted on
if ((KappaData(idat,2)<0) | (KappaData(idat,3)<0))
```

Appendix A: Matlab codes

```
        return;
    else
        kappasample = KappaData(idat,2:3);
    end

    KappaDataFull = [2      0      82.5
4      2      82.3
6      4      82.0
8      6      81.7
10     8      81.6

3008  3006  77.8
3010  3008  75.7
3012  3010  73.8
3014  3012  73.2
3016  3014  72.7
3018  3016  71.5
3020  3018  69.9
];
```

Appendix B

Statistical Results

All regressions and data analyses were performed using a program called SPSS.

There were 2 major data sets on which the statistical analyses were performed.

Data Set	No. of Parameters	Shifted
Data Set 1	8	No
Data Set 2	8	Yes

Tables B.1.1-B.1.4 represent the results obtained when regressing the unshifted data set based on all eight parameters (Data Set 1).

Descriptive Statistics

	Mean	Std. Deviation	N
KAPPA	76,1556	6,87779	2198
TI3012	113,9333	20,16917	2198
TI3126	140,5779	8,36652	2198
TI3108	132,2080	8,67394	2198
TI3100	137,5615	5,98445	2198
FFIC3105	2669,632	458,39780	2198
FFIC3112	2651,874	1633,995	2198

Table B.1.1 Representing the descriptive statistics

Appendix B: Statistical Results

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate	Change Statistics				
					R Square Change	F Change	df1	df2	Sig. F Change
1	,323 ^a	,104	,102	6,51797	,104	42,544	6	2191	,000

a. Predictors: (Constant), FFIC3112, TI3108, TI3012, FFIC3105, TI3100, TI3126

Table B.1.2 Representing the model summary

ANOVA^b

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	10844,67	6	1807,445	42,544	,000 ^a
	Residual	93082,28	2191	42,484		
	Total	103927,0	2197			

a. Predictors: (Constant), FFIC3112, TI3108, TI3012, FFIC3105, TI3100, TI3126

b. Dependent Variable: KAPPA

Table B.1.3 Representing the ANOVA table

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.	Correlations			Collinearity Statistics	
		B	Std. Error	Beta			Zero-order	Partial	Part	Tolerance	VIF
1	(Constant)	87,083	6,134		14,196	,000					
	TI3012	3,55E-02	,007	,104	5,103	,000	,089	,108	,103	,983	1,017
	TI3126	,168	,030	,204	5,679	,000	-,110	,120	,115	,317	3,159
	TI3108	-,114	,016	-,144	-6,970	,000	-,177	-,147	-,141	,955	1,047
	TI3100	-,210	,034	-,183	-6,221	,000	-,232	-,132	-,126	,473	2,113
	FFIC3105	9,79E-04	,000	,065	3,065	,002	,006	,065	,062	,901	1,110
	FFIC3112	1,07E-03	,000	,255	6,720	,000	,192	,142	,136	,283	3,529

a. Dependent Variable: KAPPA

Table B.1.4 Representing the regression coefficients

Appendix B: Statistical Results

Tables B.2.1–B.2.4 represent the results obtained when regressing the shifted data set based on all eight parameters (Data Set 2).

Descriptive Statistics

	Mean	Std. Deviation	N
KAPPA	76,1550	6,88087	2196
TI3012	113,9345	20,17831	2196
TI3126	140,5816	8,36940	2196
TI3108	132,2041	8,67692	2196
TI3100	137,5621	5,98715	2196
FFIC3105	2670,023	458,42247	2196
FFIC3112	2652,833	1634,430	2196
CHIPMOIS	54,1890	1,58444	2196

Table BC.2.1 Representing the descriptive statistics

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate	Change Statistics				
					R Square Change	F Change	df1	df2	Sig. F Change
1	,349 ^a	,122	,119	6,45932	,122	43,264	7	2188	,000

a. Predictors: (Constant), CHIPMOIS, TI3012, TI3108, TI3126, FFIC3105, TI3100, FFIC3112

Table B.2.2 Representing the model summary

ANOVA^b

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	12635,67	7	1805,096	43,264	,000 ^a
	Residual	91289,66	2188	41,723		
	Total	103925,3	2195			

a. Predictors: (Constant), CHIPMOIS, TI3012, TI3108, TI3126, FFIC3105, TI3100, FFIC3112

b. Dependent Variable: KAPPA

Table B.2.3 Representing the ANOVA table

Appendix B: Statistical Results

Coefficients^a

Model	Unstandardized Coefficients		Standardized Coefficients	t	Sig.	Correlations			Collinearity Statistics	
	B	Std. Error	Beta			Zero-order	Partial	Part	Tolerance	VIF
1 (Constant)	109,776	7,286		15,066	,000					
TI3012	3,56E-02	,007	,104	5,161	,000	,089	,110	,103	,982	1,018
TI3126	,200	,029	,243	6,815	,000	-,104	,144	,137	,317	3,158
TI3108	-,122	,016	-,154	-7,528	,000	-,177	-,159	-,151	,956	1,046
TI3100	-,168	,034	-,146	-5,016	,000	-,220	-,107	-,101	,471	2,122
FFIC3105	7,72E-04	,000	,051	2,423	,015	,006	,052	,049	,891	1,122
FFIC3112	1,34E-03	,000	,319	8,432	,000	,192	,177	,169	,281	3,558
CHIPMOIS	-,591	,089	-,136	-6,622	,000	-,120	-,140	-,133	,951	1,052

a. Dependent Variable: KAPPA

Table B.2.4 Representing the regression coefficients

Appendix C

Statistical Results From Jagarnath & Joseph

In their study, Jagarnath and Joseph (2004) added two more parameters to the model, giving then nine parameters to the model.

There were 4 major data sets on which the statistical analyses were performed . They can be represented as follows:

Data Set	No. of Parameters	Shifted
Data Set (1)	9	No
Data Set (2)	9	Yes

Descriptive Statistics			
	Mean	Std. Deviation	N
KAPPA	75.9945	8.43373	181
TI3012	111.4801	2.61303	181
TI3126	147.3022	10.50200	181
TI3108	139.1895	74.87222	181
TI3100	144.8569	3.09997	181
FFIC3105	3244.0475	906.64436	181
FFIC3111	4743.8304	485.05114	181
FFIC3001	893.0370	79.34237	181
FEED_RAT	7.6680	1.58950	181
CHIP_MOI	53.8790	1.94073	181

Table C.1.1: Representing the Descriptive Statistics obtained for Data Set (1)

Appendix C: Statistical Results

Model Summary									
Model	R	R Square	Adjusted R Square	Std. Error of the Estimate	Change Statistics				
					R Square Change	F Change	df1	df2	Sig. F Change
1	.420 ^a	.176	.133	7.85374	.176	4.063	9	171	.000

a. Predictors: (Constant), CHIP_MOI, FEED_RAT, TI3108, TI3012, TI3126, FFIC3111, FFIC3105, TI3100, FFIC3001

Table C.1.2: Representing the model summary obtained for Data Set (1)

ANOVA ^b						
Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	2255.507	9	250.612	4.063	.000 ^a
	Residual	10547.488	171	61.681		
	Total	12802.994	180			

a. Predictors: (Constant), CHIP_MOI, FEED_RAT, TI3108, TI3012, TI3126, FFIC3111, FFIC3105, TI3100, FFIC3001
b. Dependent Variable: KAPPA

Table C.1.3 Representing the ANOVA table obtained for Data Set (1)

Coefficients ^a									
Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.	Correlations		
		B	Std. Error	Beta			Zero-order	Partial	Part
1	(Constant)	3.660	36.948		.099	.921			
	TI3012	.047	.243	.014	.192	.848	.095	.015	.013
	TI3126	.149	.061	.186	2.464	.015	.265	.185	.171
	TI3108	.001	.008	.012	.162	.871	.002	.012	.011
	TI3100	.281	.224	.103	1.258	.210	-.004	.096	.087
	FFIC3105	-.001	.001	-.129	-1.681	.095	-.086	-.127	-.117
	FFIC3111	-.001	.001	-.071	-.826	.410	.070	-.063	-.057
	FFIC3001	.034	.010	.315	3.406	.001	.219	.252	.236
	FEED_RAT	-1.247	.438	-.235	-2.845	.005	-.219	-.213	-.197
	CHIP_MOI	-.119	.311	-.027	-.383	.702	.029	-.029	-.027

a. Dependent Variable: KAPPA

Table C.1.4 Representing the regression coefficients obtained for Data Set (1)

Descriptive Statistics			
	Mean	Std. Deviation	N
KAPPA	76.2584	7.93907	178
TI3012	111.2685	2.35922	178
TI3126	146.4090	10.98385	178
TI3108	139.1730	75.50106	178
TI3100	144.7404	3.11772	178
FFIC3105	3226.3236	891.02474	178
FFIC3111	4744.0933	488.87667	178
FFIC3001	891.6781	79.17018	178
FEED_RAT	7.6303	1.57199	178
CHIP_MOI	53.8590	1.94624	178

Table C.2.1: Representing the Descriptive Statistics obtained for Data Set (2)

Model Summary									
Model	R	R Square	Adjusted R Square	Std. Error of the Estimate	Change Statistics				
					R Square Change	F Change	df1	df2	Sig. F Change
1	.431 ^a	.186	.142	7.35256	.186	4.263	9	168	.000

a. Predictors: (Constant), CHIP_MOI, TI3126, TI3108, TI3100, FFIC3105, TI3012, FFIC3111, FEED_RAT, FFIC3001

Table C.2.2 : Representing the model summary obtained for Data Set (2)

ANOVA ^b						
Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	2074.014	9	230.446	4.263	.000 ^a
	Residual	9082.098	168	54.060		
	Total	11156.112	177			

a. Predictors: (Constant), CHIP_MOI, TI3126, TI3108, TI3100, FFIC3105, TI3012, FFIC3111, FEED_RAT, FFIC3001

b. Dependent Variable: KAPPA

Table C.2.3 :Representing the ANOVA table obtained for Data Set (2)

Appendix C: Statistical Results

Coefficients^a									
Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.	Correlations		
		B	Std. Error	Beta			Zero-order	Partial	Part
1	(Constant)	-29.113	38.753		-.751	.454			
	TI3012	.049	.251	.015	.196	.845	.081	.015	.014
	TI3126	.115	.053	.159	2.143	.034	.229	.163	.149
	TI3108	.004	.007	.036	.511	.610	.005	.039	.036
	TI3100	.412	.209	.162	1.976	.050	.011	.151	.138
	FFIC3105	.000	.001	-.053	-.680	.498	-.010	-.052	-.047
	FFIC3111	-.002	.001	-.124	-1.442	.151	.082	-.111	-.100
	FFIC3001	.039	.009	.394	4.420	.000	.287	.323	.308
	FEED_RAT	-1.200	.427	-.238	-2.809	.006	-.172	-.212	-.196
	CHIP_MOI	.148	.289	.036	.512	.610	.066	.039	.036

a. Dependent Variable: KAPPA

Table C.2.4: Representing the regression coefficients obtained for Data Set (2)

Based on the regression of nine parameters, study realized by two students at University of KwaZulu-Natal, we can observe that the parameter of the Tag TI 3108 is not relevant as it yielded the smallest value of the Zero-order and Partial correlation coefficients.

			Correlation Coefficients			
			Unshifted data		Time shifted data	
No.	Parameter	Tag No.	Zero Order	Partial	Zero Order	Partial
1	Top Circ Temp	TI 3012	0.09524	0.01469	0.08064	0.01508
2	Dig Phase Temp	TI 3126	0.26451	0.18519	0.22926	0.16315
3	Circ Temp Before C8	TI 3108	0.00228	0.01239	0.00511	0.03943
4	Temp Adj Before C6	TI 3100	-0.00379	0.09579	0.01140	0.15074
5	Upper Circ Flow	FFIC 3105	-0.08595	-0.12749	-0.00971	-0.05238
6	Wash Dig Nozzle	FFIC 3111	0.06976	-0.06306	0.08241	-0.11056
7	White Liquor Flow	FFIC 3001	0.21937	0.25205	0.28677	0.32276
8	Chip Revs	C 30	-0.21883	-0.21256	-0.17157	-0.21178
9	Chip moisture content	-	0.02888	-0.02926	0.06621	0.03944