Institute of Paper Science and Technology

MAPPS PERFORMANCE ATTRIBUTE SYSTEM

Project 3471

REPORT THREE

to

MEMBER COMPANIES OF
THE INSTITUTE OF PAPER SCIENCE AND TECHNOLOGY

August 1991

Atlanta, Georgia

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Institute of Paper Science and Technology
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MAPPS Performance Attribute System

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Report 3

To

Member Companies of the Institute of Paper Science and Technology

By

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August 1991

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PERFORMANCE ATTRIBUTES

INTRODUCTION

Performance attribute modeling (PAT modeling) is a novel extension of the MAPPS simulation package. Release Version 3.0 of MAPPS incorporated the use of a second stream structure - the performance attribute stream. With Release Version 4.0, however, the PAT modeling capabilities of MAPPS have been greatly extended.

The term "performance attribute" refers to properties and characteristics of fibrous process streams that are "nonconserved," as opposed to "conserved" properties like mass and energy flows. A "performance attribute stream" thus consists of an array of parameters containing a well-defined set of such nonconserved properties. Examples of performance attribute parameters are pulp kappa number, pulp freeness, fiber length and width distributions, and fiber cell-wall thickness. The PAT stream structure makes it possible to transfer important nonconserved properties of a fibrous stream from one MAPPS module to another in addition to the mass and energy flows transferred in the regular MAPPS streams. Since the PAT stream definition only contains properties typical for fibrous process streams, it can only exist parallel to MAPPS stream types 3, 5, or 6 (i.e., pulp, bleaching, or paper streams).

The term "PAT modeling" refers to simulation in MAPPS where theoretical models are used which not only calculate mass and energy balances but also calculate different pulp or paper properties with help of information carried in the PAT stream.

POTENTIAL BENEFITS

PAT modeling has the potential of improving decision-making in pulp and paper manufacturing. PATS give MAPPS the ability to create a simulation model where raw materials and processing steps can be manipulated to produce a paper product with a set of specified end-use characteristics. PAT modeling offers a host of opportunities for optimization of the paper manufacturing process, including significant opportunities for reduced energy consumption in an energy-intensive industry. *Some potential benefits with energy implications include:*

1) Reduced energy consumption through increased use of recycled and high-yield furnishes;
2) Reduced energy consumption through reduced fiber loss in manufacturing;
3) Reduced energy consumption by eliminating off-specification product and the subsequent recycle of the off-spec product;
4) Reduced energy use through optimization of processing steps for a given product specification;
5) Improved decision-making in process selection and capital equipment selection.

OVERVIEW

Property Development During Papermaking

Pulp and paper manufacturing is a process for which the original raw material is wood chips from one or more species, and the final product is a certain pulp or paper grade with a certain set of desired end-use performance characteristics or specifications. In general the end-use specifications are dependent on the grade being produced. In the overall process, the wood chip fibers may be separated by mechanical or chemical means, processed to enhance their bonding potential, formed into sheets, pressed to consolidate and remove water, dried and passed through a variety of converting operations to achieve the final slate of properties.

Conventional process simulation techniques treat the pulp and paper manufacturing process as a flow of mass and energy only. Fibers are viewed simply as lumped components of cellulose and lignin or as generic fibers. Neither the structure of the fibers, nor the network the fibers form are taken into account. Important interactions between fiber or network properties and mass and energy balances, particularly in sheet forming and dewatering, are thus impossible to represent with conventional process simulation techniques.

A considerable body of knowledge has been developed relating characteristics of fibers and fiber networks with final paper sheet properties. Until recently, this information has been underutilized in general, and it has been almost totally ignored in the areas of process simulation and modeling.

The work of many authors has established a sound theoretical framework of the structure of paper and models of many sheet properties (27-37). Relevant areas of fiber and sheet structure, optical properties, and process effects have been extensively reviewed (47-60). Others have contributed knowledge on the wide variety of factors which influence fiber and network properties such as species, sheet forming, wet consolidation, stretch and orientation, and pulping (9-26,38-46,61-69).

The MAPPS PAT system now provides the means of linking these more fundamental models for sheet properties with basic fiber and network properties and processing conditions. As shown in Figure 1, performance attributes (PATs) are fundamental variables of the fibers and network which link raw materials and processing conditions (represented by "process attributes" in the figure) to various measures of end-use performance of paper products.

Figure 2 illustrates how mass and energy balance models, PAT models and paper property models interact in MAPPS. The models are input-output in nature, so the mass and energy flows and performance attributes entering a processing step are changed before leaving, depending on the characteristics of the processing step. Performance attributes of the entering and leaving streams along with material flow information are used to determine properties of the streams entering and leaving each operation block.

FIGURE 1 - RELATIONS BETWEEN PROCESS AND PERFORMANCE ATTRIBUTES

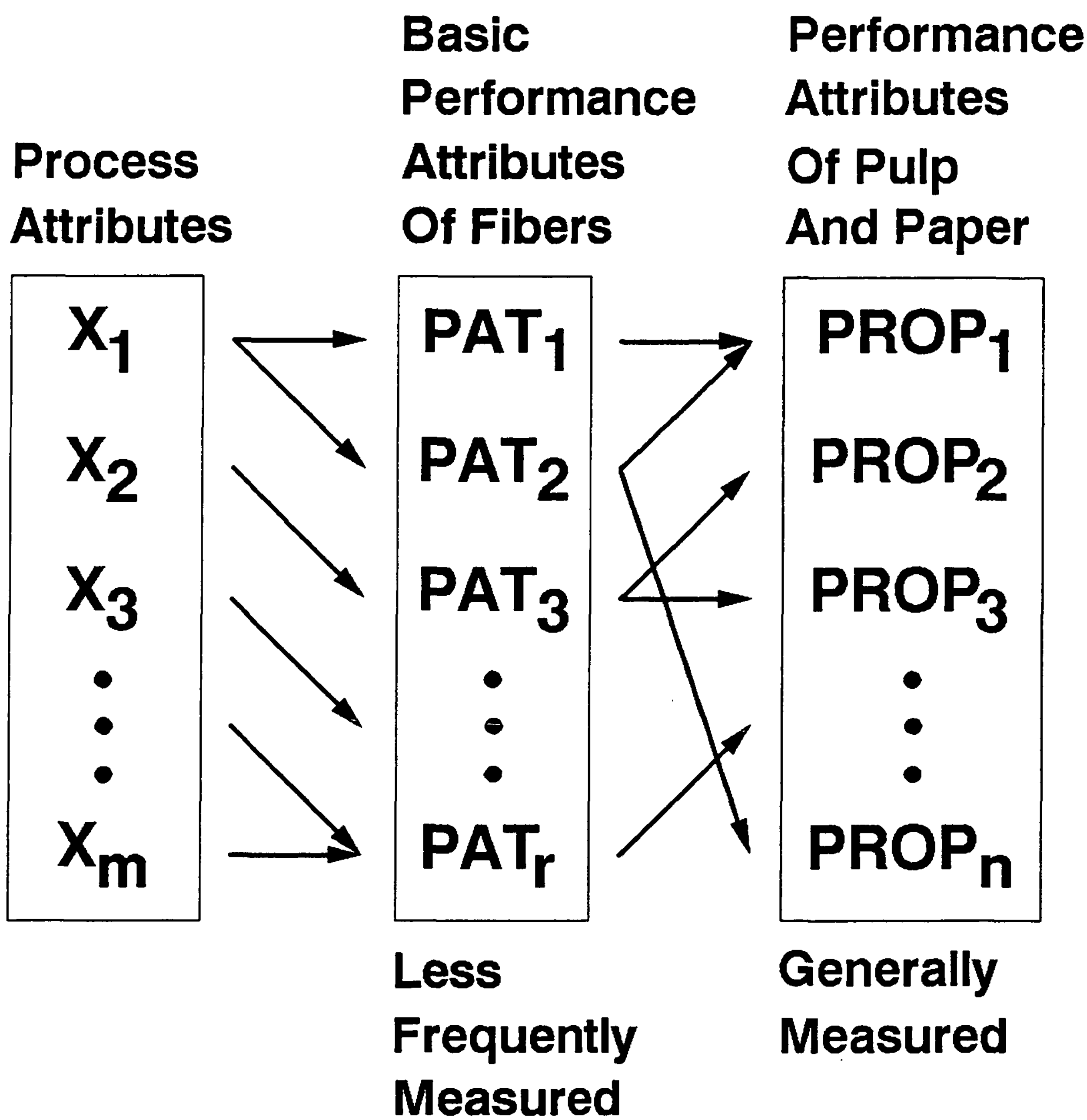
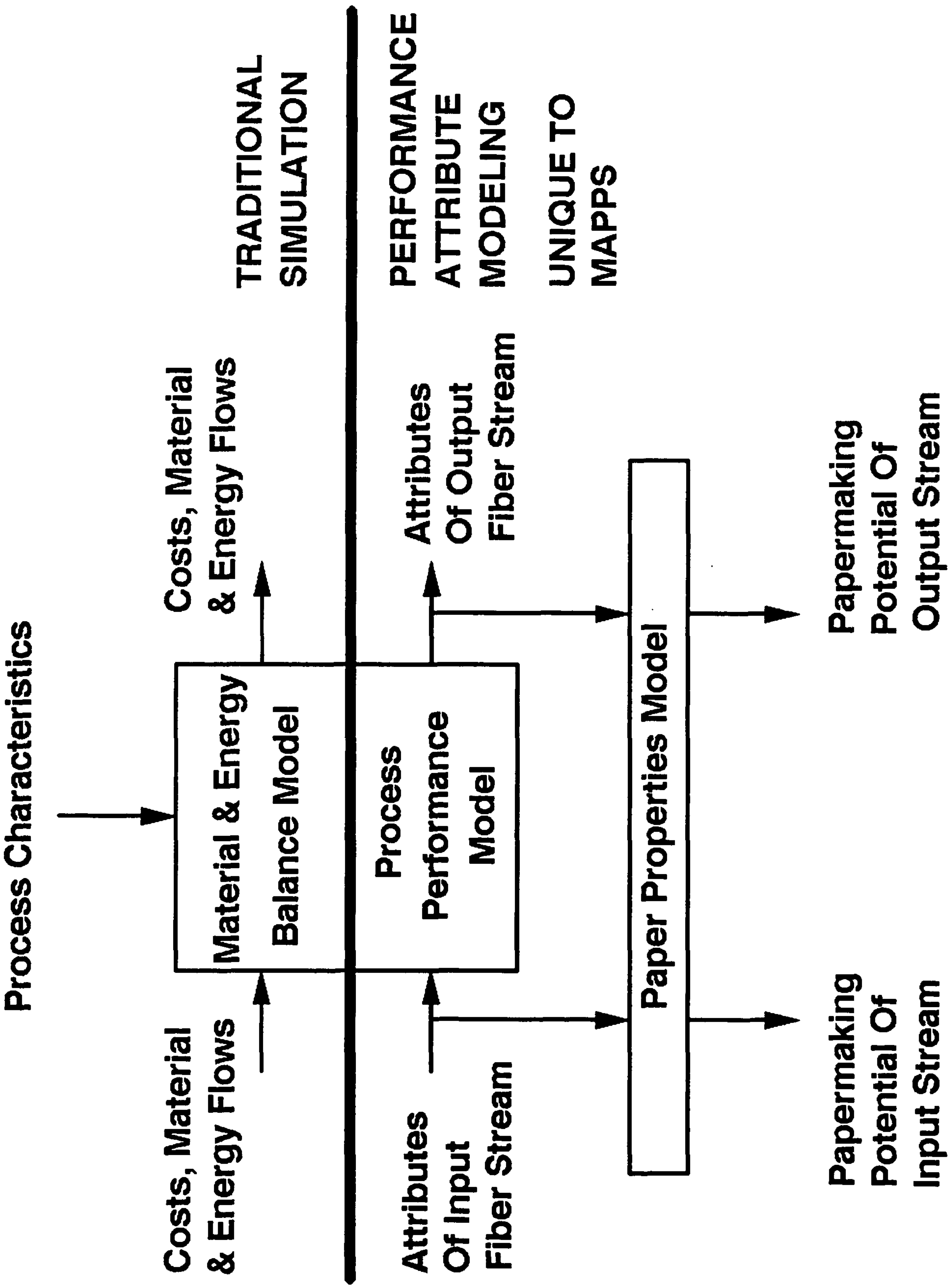


FIGURE 2 - INTERACTION BETWEEN TRADITIONAL MASS AND ENERGY MODELS AND PAT MODELS



The approach to PAT modeling is the same as for "standard" MAPPS simulation. A model of the process to be simulated must be assembled based on flow diagrams, etc. (see Section 2 of the MAPPS User's Guide). Figure 3 shows a diagram of a process model developed for a high-yield pulping process.

Simulation of the process model then provides information on the development of various properties and performance attributes throughout the process. Figure 4 illustrates the development of some handsheet properties at different stages of the high yield pulping process in Figure 3.

The PAT system must account for a wide range of factors which influence end-use properties. Examples include wood species used, pulping and bleaching conditions, screening and cleaning procedures, additives used, sheet forming, wet stretching, pressing, drying, calendering, and repulping.

The PAT system accounts for wood species through the use of a species database. When initializing a chip or pulp flow, the user can specify the species he wants to simulate, and a set of default performance attribute parameters for that particular species will be retrieved from the species database. The remaining, process-dependent factors will be accounted for in the theoretical models for each unit operation, where the effect of the particular process on each performance attribute parameter is modeled.

Parameters

This section provides an overview of the individual performance attribute parameters and how they are affected by various processing conditions. Figure 5 illustrates how the performance attributes represent the various aspects of fibers and network which constitute paper.

PATs Related to Chemical Composition

Performance Attribute	Symbol
Yield..	YIELD
Kappa Number...................................	KAPPA
Ratio of Hemicellulose to Total Cellulose.....	XHEMI

Fibers consist of alpha-cellulose, hemicellulose, lignin, extractives, and ash. However, for convenience the attributes used to represent fiber composition are yield, kappa number and the ratio of hemicellulose to total cellulose. The pulp stream in MAPPS (type 3) carries the total amount of cellulose as one of its chemical components. By having the hemicellulose-to-cellulose ratio specified as a PAT parameter, it is possible to calculate the actual amounts of alpha-cellulose and hemicellulose in a pulp stream.

FIGURE 3 - PROCESS MODEL OF A HIGH YIELD PULPING PROCESS

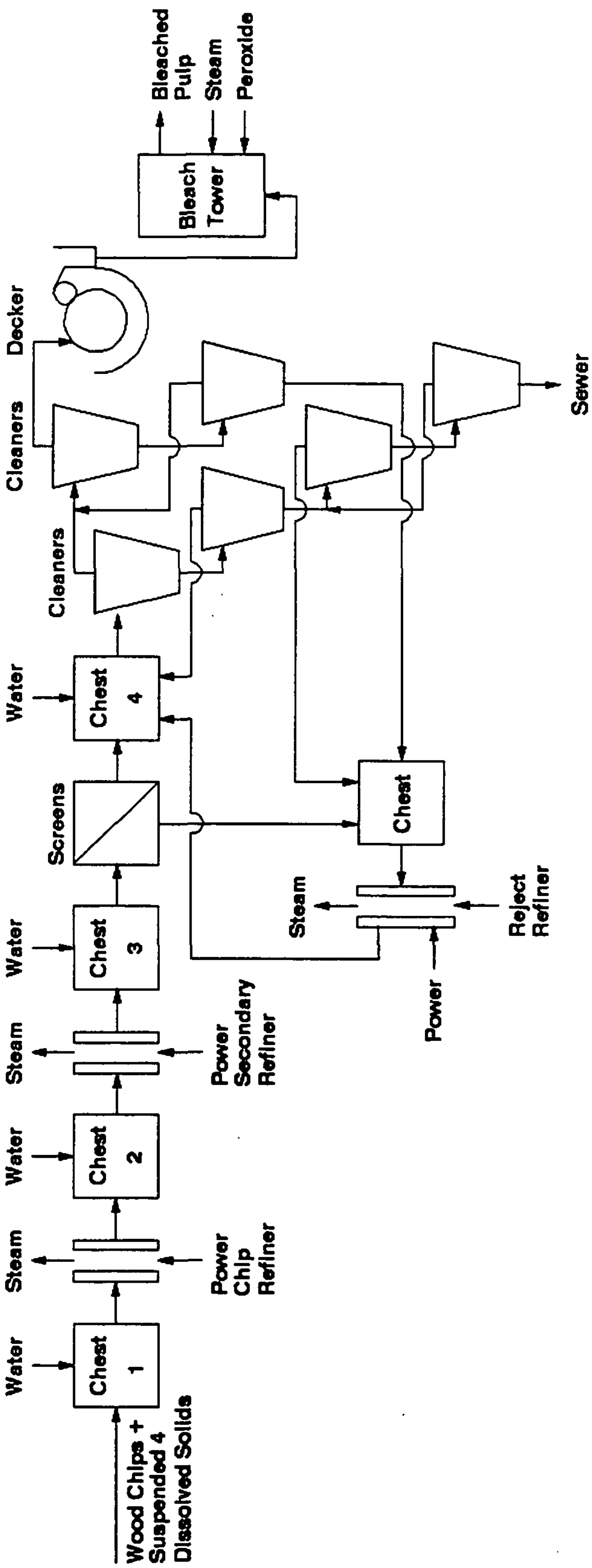


FIGURE 4 - DEVELOPMENT OF PAPER PROPERTIES

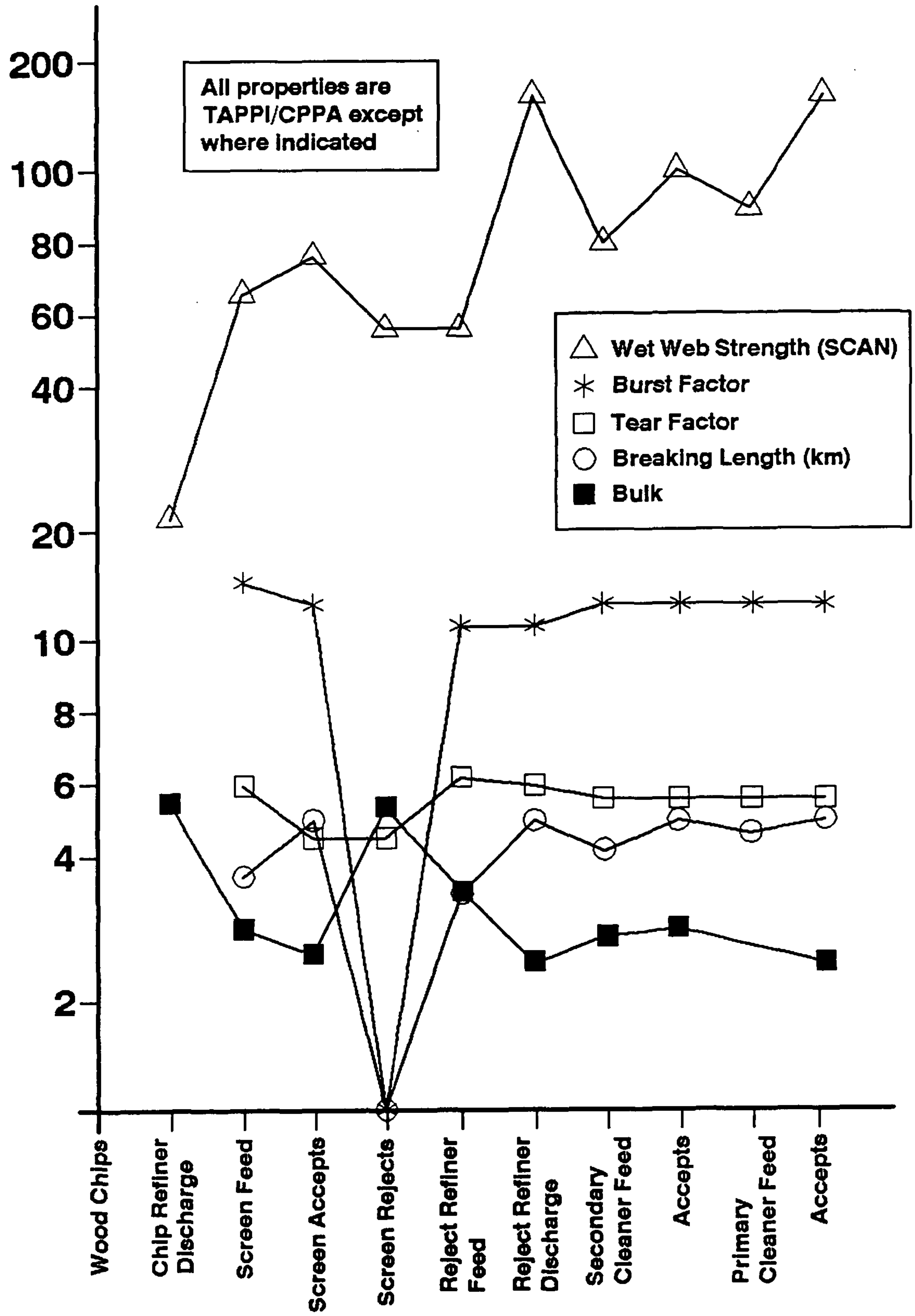
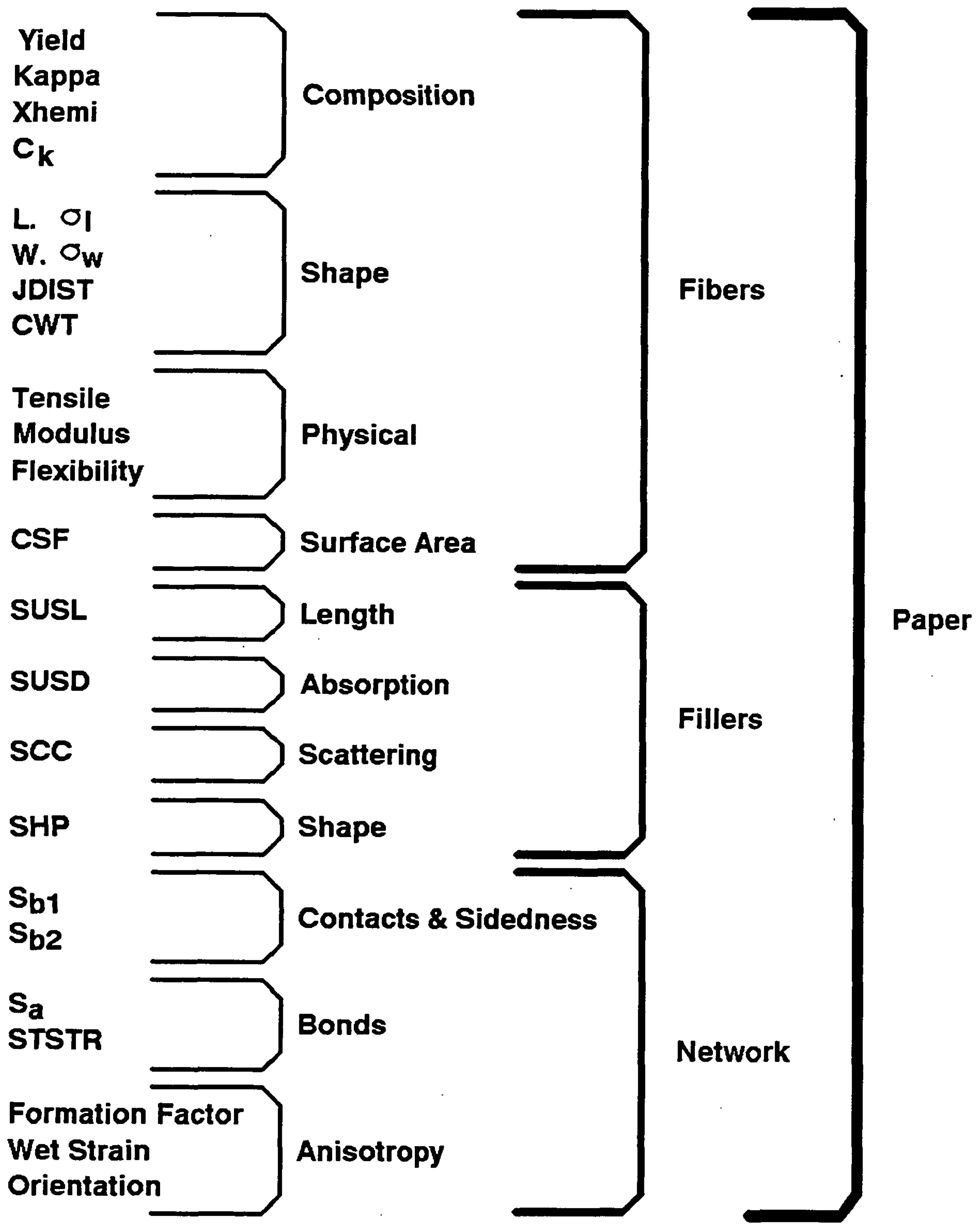


FIGURE 5 - OVERVIEW OF PAT PARAMETERS IN MAPPS



The kappa number is assumed to be linearly related to the lignin content of the fiber. In MAPPS, this linear relationship is as follows: Kappa number = 660 * lignin content. With the variables listed above, it is thus possible to determine the chemical composition of fibers, assuming the extractives have been removed. These three attributes account for many of the primary effects of pulping. Other effects are discussed in the section on pulping.

PATs Related to Optical Attributes

Performance Attribute	Symbol
Absorption Coefficient........................	C_k

The light absorption coefficient is an inherent characteristic of the lignin color bodies in the fiber. This attribute is influenced by lignin removal steps such as pulping and bleaching. A second optical property, the light scattering coefficient, can be predicted from other sheet characteristics. Sheet brightness, an important end-use performance characteristic of many paper grades, can then be predicted through use of the Kubelka-Munk theory, where sheet brightness is assumed to be a function of the scattering and absorption coefficients. For paper grades containing fillers, the brightness depends on the scattering and absorption coefficient of both the fibers and fillers.

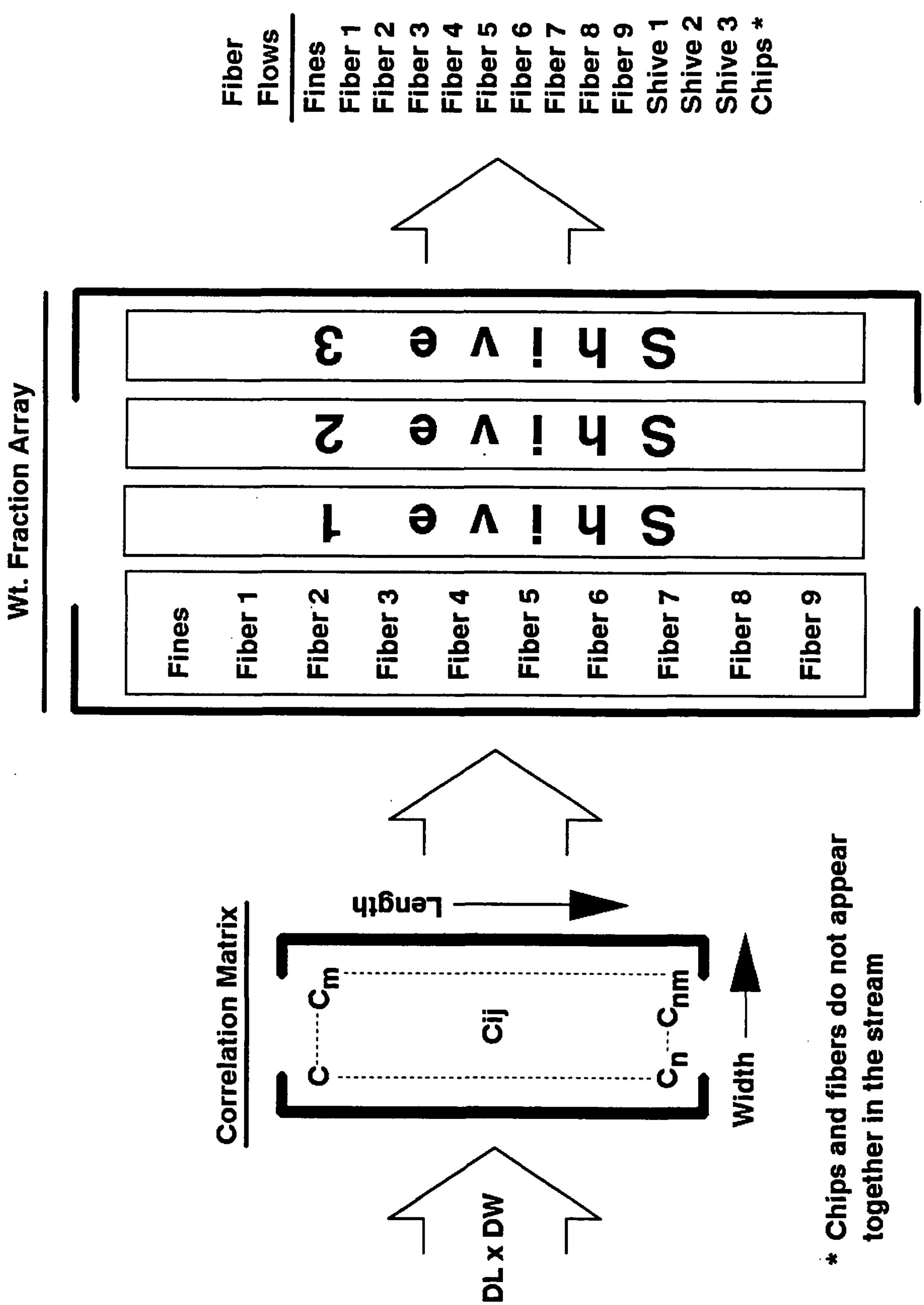
Brightness development is accomplished through various types of bleaching operations. Bleaching can also have beneficial effects on other properties through the removal of lignin. The three attributes, yield, kappa and absorption coefficient can be used to account for the main effects of bleaching.

PATs Related to Fiber Shape

Performance Attribute	Symbol
Average Fiber Length..........................	L.
Standard Deviation of Fiber Length............	σ_l
Average Fiber Width...........................	W.
Standard Deviation of Fiber Width.............	σ_w
Distribution Type.............................	JDIST
Cell Wall Thickness...........................	CWT

Fiber shape or morphology is represented by fiber length and width distributions and cell wall thickness. The length and width distribution are represented by the average and the standard deviation. A third parameter, the distribution type: IDIST, defines the type of distribution. At present, there are four types of distributions the user can choose between: log-normal, normal, Weibull, and modified log-normal distribution.

FIGURE 6 - MAPPING OF 100 INTERNAL FIBER TYPES TO 13 PAPER STREAM COMPONENTS



By combining the discrete distribution functions for fiber length and width DL and DW through multiplication into a correlation matrix as shown in Figure 6, it is possible to represent all combinations of fiber length and width. Each portion of the correlation matrix is assigned to a specific fiber category, where each fiber category represents fibers of a certain length and/or width. Currently, there are 13 fiber categories defined in MAPPS: FINES, FIBER TYPE 1-9, and SHIVES TYPE 1-3. Each fiber category (including fines is defined over a small range of length and width. All fibers are defined over the same narrow fixed width range. Each shive component represents a specific width range but is independent of length.

The species database contains default values for the fiber shape attributes for each species in their native state (i.e., for unpulped wood chips). Throughout a simulation the fiber length and width distributions will be shifted by various operations such as refining, screening, cleaning, and papermaking.

PATs Related to Fiber Physical Properties

Performance Attribute	Symbol
Specific Bond Strength........................	SBSTR
Fiber Tensile Strength........................	Tensile
Fiber Modulus.................................	Modulus
Fiber Stiffness Factor........................	Flexibility

Important physical properties are fiber specific bond strength, tensile strength, and fiber modulus.

SBSTR, specific bond strength, refers to the strength developed between fibers per unit weight of fibers when bonds are formed. SBSTR is a function of the chemical and physical makeup of the outside surface of fibers and thus depends on wood species and the pulping and bleaching conditions used. Tensile strength is defined as the weight required to cause axial failure in a fiber divided by the original cross sectional area. The tensile strength is usually converted to a breaking length since the tensile strength of individual fibers is rarely measured. A more common operating measurement is the zero-span tensile test; however, at low levels of refining and pulping, this measurement may not always represent intrinsic fiber strength.

Fiber modulus (or tensile modulus) is the initial slope of the stress-strain curve and is thus a measure of the axial stiffness of the fiber. These properties are not easily measured but they are extremely influential in determining final sheet properties. Future research efforts will likely result in models for both axial and transverse fiber modulus.

A fiber property which contributes significantly to bonding potential is fiber compliance or bending stiffness. Fiber stiffness tends to increase with increased cell wall thickness, increased yield (more lignin present) and a decreased degree of refining (less swelling or removal of the outermost layer of the fiber). The effect of these factors are generally already accounted for by the performance attributes previously mentioned, with the major exception of drying effects. When fibers are dried, they become stiffer and some fiber fractions do not return to their predried condition upon rewetting. This effect, sometimes referred to as hornification, is particularly important in the simulation of fiber repulping and secondary fiber use. It is accounted for by the use of a fiber stiffness factor, SMOD, which increases when the fibers are dried above a critical level (93%). Upon subsequent refining or bleaching, this factor is reduced by an appropriate amount to qualitatively simulate the restoration of fiber flexibility to its predried state. SMOD may also be specified differently from the default value of one to account for uncertainties in cell-wall thickness, CWTH.

The species database contains default values for these attributes for each of the species represented.

PATs Related to Fiber Surface Area

Performance Attribute	Symbol
Canadian Standard Freeness....................	CSF

Due to the extensive fibrillate structure of wood fibers, the actual external surface area is generally larger than would be expected for smooth cylinders. External surface area is developed extensively by refining and is a critical step in papermaking. The attribute Canadian Standard Freeness, CSF, accounts for these effects and is assumed to be related to the hydrodynamic specific surface area of the fiber.

The fiber length distribution determines the fraction of fines and fibers in the pulp furnish. However, for any given fiber length, the degree of surface area development can vary and is handled internally to MAPPS by a new factor called the K-factor (unrelated to kappa number). Given the fiber length distribution parameters (average fiber length; AVGL, and fiber length standard deviation; SIGL) plus the K-factor, one can compute the hydrodynamic specific surface area, Sh. Given Sh, it is then possible to determine CSF. Therefore, knowing any three of the four quantities, AVGL, SIGL, K-factor, and CSF, the remaining quantity can be computed. In MAPPS, AVGL, SIGL, and CSF are the properties passed by the performance attribute stream vector, while the K-factor and the hydrodynamic specific surface area, Sh, are computed internally.

Two important effects of refining, fiber separation and surface area development, are accounted for through the use of the fiber length distribution parameters, AVGL and SIGL, and Canadian Standard Freeness, CSF. Other effects of refining, such as swelling, increased fiber flexibility and bonding potential are accounted for by factors discussed later.

PATs Related to Network Formation

Performance Attribute	Symbol
Potential Bonded Area, Top................	S_{b1}
Potential Bonded Area, Bottom............	S_{b2}
Actual, Relative Bonded Area.............	S_a
Formation Coefficient....................	Formation Factor
Wet Stretch (MD).........................	Wet Strain
Fiber Orientation Ratio..................	Orientation

Once the fibers have been separated and their surface area has been developed through refining, the stage is set for sheet forming, i.e., network formation. The major functions of any sheet forming process, such as the fourdrinier, twin-wire former, or handsheet former, is to form a web of fibers from a dilute stock and drain as much water as possible from this formed paper web. Inevitably, much of the fines, small fibers, and suspended material in the original stock flow will not be contained in the paper web but will drain through the web with the water. Thus, the sheet that is eventually formed contains a different fiber makeup than the stock entering the forming device.

Also, the fiber laydown mechanism of each forming process imparts a variability to the fiber network called anisotropy. A paper sheet is not perfectly uniform and variability occurs in mass distribution from point to point in the plane of the sheet due to flocculation of fibers. This variability is referred to as formation; i.e. the better the formation, the less the variability. Fibers tend to be oriented preferentially in the machine direction due to the speed differential between the jet and the wire and the sheet is preferentially strained in the machine direction due to slight differences in speed along the machine. Both of these processes lead to built-in anisotropic stress distribution, which causes directionally dependent properties in all three directions, MD, CD, and ZD. In addition, variability in fiber retention during forming leads to ZD variability and sidedness.

FIBER/NETWORK BOND DEVELOPMENT

Fiber/network bond development may be discribed as the generation or Loss of Optical Contact Through Forming, Wet Pressing, Drying, and Converting operations

Sheet Forming

As each layer of fibers is deposited during the sheet forming process, fiber contacts are established. Initially, the contact areas are relatively few due to the low consolidation forces and the high moisture content of the mat. As moisture is removed and pressure applied, fiber-fiber contact increases through mechanical and surface tension forces (Figure 7). Variable the potential relative bonded area, SBO, occurs as a result of the fiber contact generated during forming and prior to pressing. SBO is a function of two factors: the hydrodynamic specific surface area (related directly to CSF) and fiber flexibility. Both of these parameters are functions of fiber species, refining and previous pulping conditions.

As the fiber mat develops along the wire, fiber and particle retention increases. The fiber length distribution tends to shift as a result of the increased retention of fines on the upper layers of the mat and the loss of fines from the wire side of the sheet. In twin-wire systems, this retention behavior is more symmetrical since dewatering occurs from the top & bottom of the sheet but the principles still apply. Thus distribution of fiber length differs throughout the thickness of the sheet leading to a z-directional variation in fiber-fiber contacts.

In order to pass this ZD contact structure on to other process modules, the contact areas of the top and bottom of the sheet are passed as PAT variables, SB1 and SB2, respectively. In addition, a matrix of variables, i.e., fiber length distribution parameters, freeness, K-factor and others is passed to the following modules to represent the ZD structure of the sheet. These variables help to represent some of the inherent surface and bulk characteristics of the sheet.

Wet Pressing

During pressing, additional sheet consolidation forces are applied to remove water, thus increasing the fiber-fiber contact areas (Figure 7). The PAT variables SB1 and SB2 represent fiber-fiber contact areas of the top and bottom of the sheet, either before or after pressing. Using the aforementioned matrix of structural information from the forming operation, the pressing operation increases the contact areas of each side of the sheet. Thus, SB1 and SB2 are likely to vary differently during pressing. Consequently, each press nip, represented by a WPRESS module, will tend to increase the potential bonded areas of the top and bottom of the sheet. This effect diminishes as the sheet is consolidated (dewatered) by subsequent press nips.

Sheet compressibility during pressing is a function of PAT variables namely yield, cell-wall thickness, freeness, and fiber stiffness factor. Also at sufficiently high pressures individual fiber lumens may collapse, leading to an increase in fiber modulus.

Drying - Generation of Hydrogen Bonding

Drying has two primary functions: to increase solids content to 93% or higher, and to form hydrogen bonds which increase the strength of the fiber network. As the sheet dries, areas in optical contact are converted to actual bonded area (ASB) based upon the degree of moisture removal and the temperature level. Other important factors, i.e., preferential strain in the machine direction due to lack of restraint in the cross-machine direction, can lead to undesirable effects, i.e., curl. Currently the dimensional stability effects due to variable drier restraint can not be modeled by the PAT system. The basic model for bond development through pressing and drying is illustrated in Figure 7.

FIGURE 7 - BOND DEVELOPMENT MODEL IN MAPPS

- **Fiber Property Development**

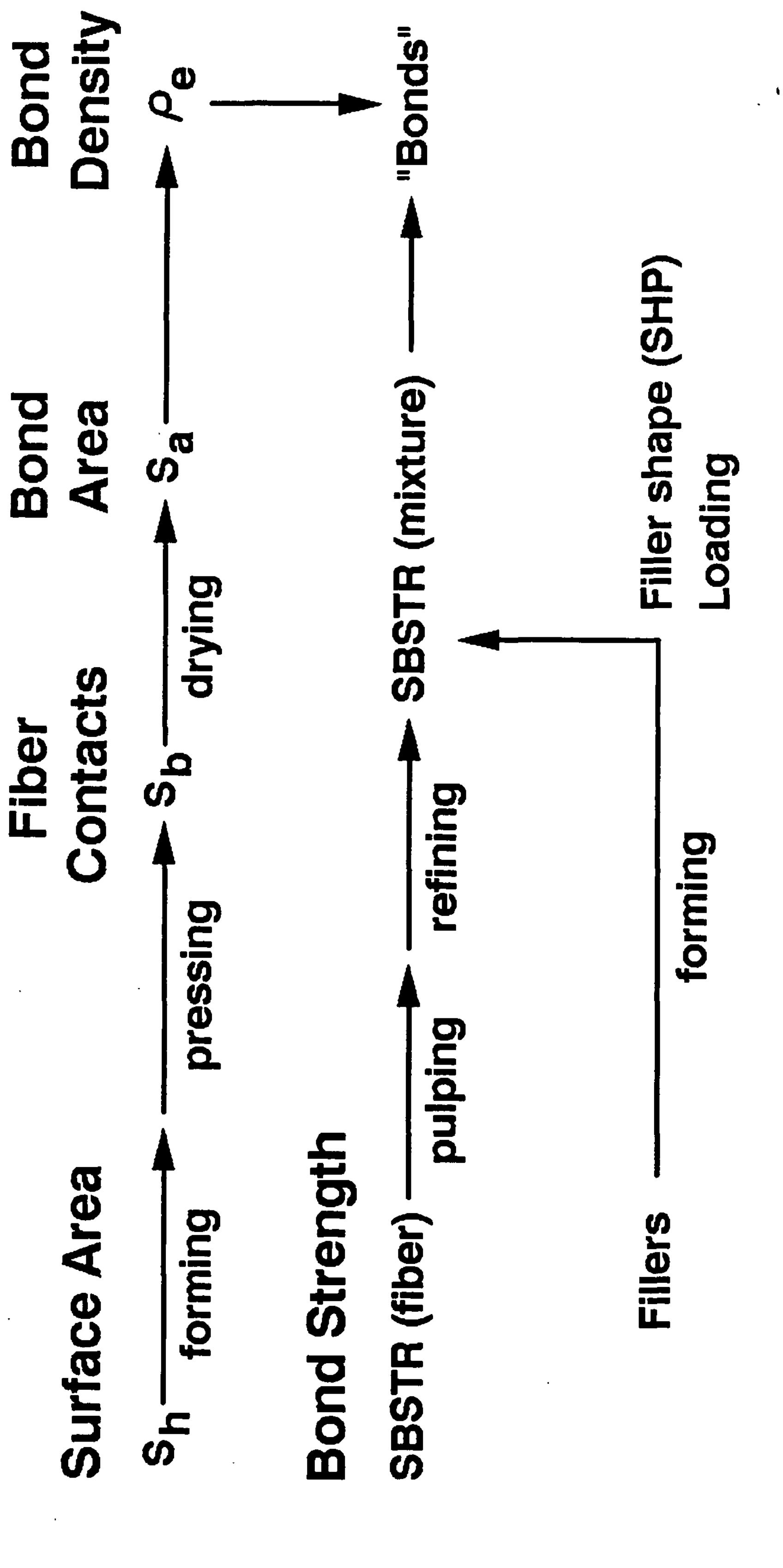
	• Refining	
• Refining	• Pulping	
• Species	• Species	
Affects ↓	Affects ↓	
Hydrodynamic Specific Surface +	Fiber Flexibility —Forming→	Potential Relative Bonded Area (SBO)

- **Sheet Consolidation**

SBO —Pressing→ SB1/SB2 —Drying→ ASB

SBO	SB1/SB2	ASB
	Potential Bonded Area Top/Bottom	Actual Relative Bonded Area

FIGURE 8 - BOND DEVELOPMENT CONCEPTS



Based upon the moisture and temperature of the drying process, a portion of the fiber-fiber contact areas, SB1 and SB2, will be converted into a bulk bond area, ASB. ASB then affects the total relative bonded area, as described in later sections. If moisture is added to the sheet, water will tend to displace some of these hydrogen bonds and ASB will decrease. Thus reslurrying of the sheet will decrease ASB to zero and the sheet properties will reflect the absence of fiber bonding.

Calendering and Other Converting Operations

During calendering, the sheet is subjected to pressure and stress distributions which will differ significantly for different types of calendering operations, i.e., soft calendering, hard-nip calendering or gloss calendering. Applied pressure during calendering can densify the sheet, thus increasing fiber-fiber contacts. The relationship between fiber contacts and density will be discussed in a later section.

Fiber Bonds and the Effects of Fillers

The concepts used to model fiber-fiber bonds are shown in Figure 8. Each bond has two parts, density and strength. As shown, fillers tend to interfere with bonding, and thus, the specific bond strength of the filled sheet, SBSTR, is reduced in direct proportion to the filler loading. The shape factor attribute of the filler, SHP, influences the slope of the line relating specific bond strength loss vs. filler loading. Other filler attributes such as size distribution, electrophilic properties, brightness, etc.,affect filler retention and the optical properties of filled sheets.

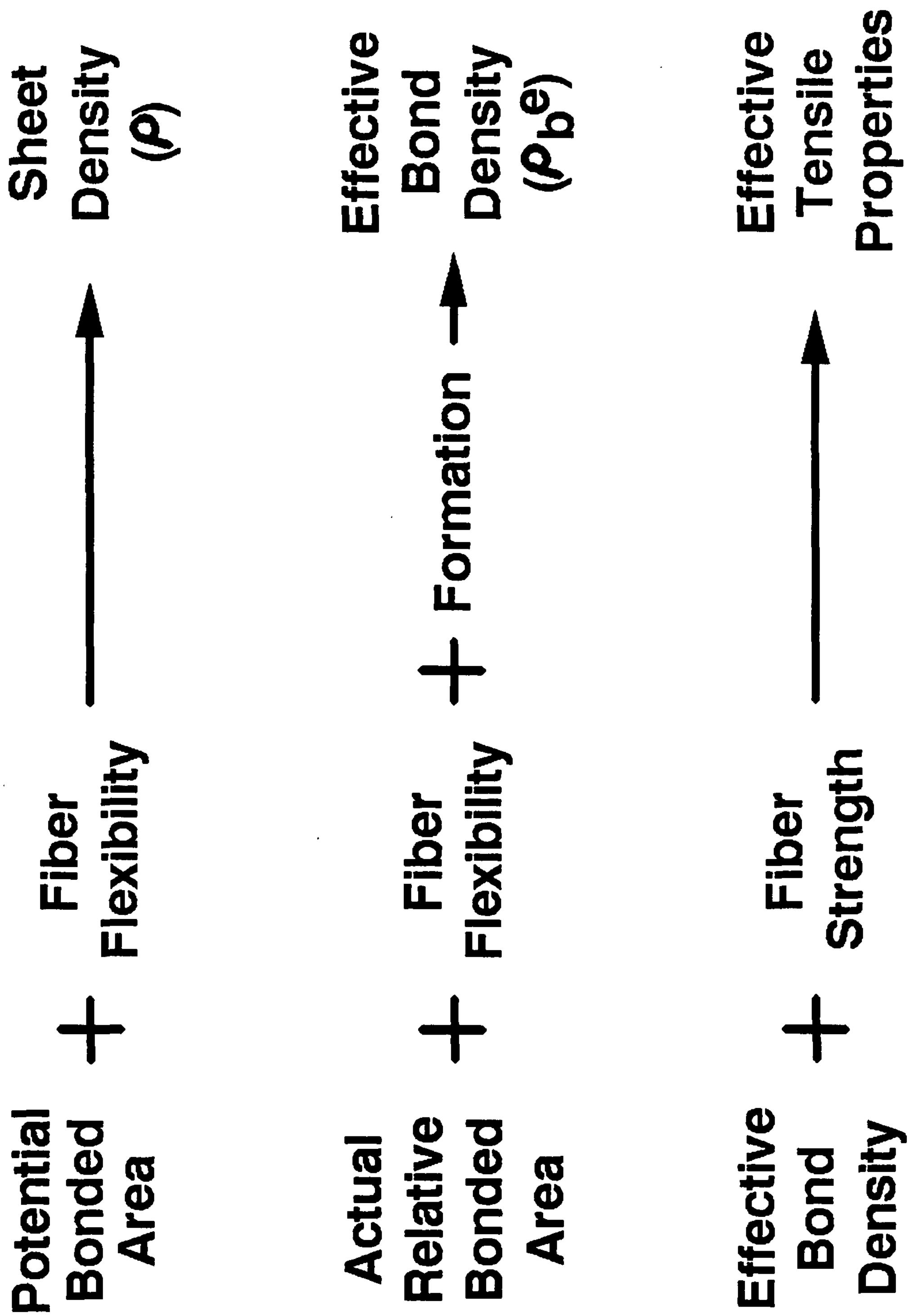
Fiber Stiffening and Cellulose Collapse During Drying

As the fiber dries, the cellulose matrix tends to collapse resulting in an increase in tensile and bending modulus (stiffness) and an apparent drop in the bonding potential of dried fibers (hornification). Thus, when dried fibers are repulped, they tend to form bulkier, weaker sheets, unless they are re-refined or pass through chemical treatments to open up the cellulose structure again. In order to simulate this stiffening effect, another PAT, the fiber stiffness factor, SMOD, is increased in the dryer in proportion to the amount of fiber drying.

Sheet Densification and Strength Development

One of the key concepts in the PAT model system is the relationship between potential bonded area and sheet density and between actual bonded area and bond density, as illustrated in Figure 9. Potential bonded area represents optical contact between fibers but this factor alone does not necessarily mean that hydrogen bonds have been formed. However, a high level of optical contact leads to high sheet density and the increased potential for conversion of optical contact surface into bonded surface, leading to bond density and sheet strength.

FIGURE 9 - SHEET DENSIFICATION AND STRENGTH DEVELOPMENT



After sheet densification by pressing, the drying operation converts the potential bonded areas of the top and bottom of the sheet, SB1 & SB2, respectively, to the actual bonded area, ASB. Within MAPPS, the value of ASB is calculated as the conversion of the average of the individual potential bonded areas, SB1 & SB2, to actual bonded area. Thus, ASB, which primarily affects tensile properties such as modulus, breaking length, etc., and SB1 & SB2, which primarily affect optical properties, particularly scattering coefficient, play a crucial role in determining the bulk properties of the sheet. The models for bulk sheet density and bond density have the same form but sheet density depends primarily on SB while bond density depends primarily on ASB. For perfectly formed dry sheets, sheet density and bond density will be the same and sheet tensile properties will correspond to sheet density. However, as sheet anisotropy increases, the effective bond density decreases, thus decreasing the sheet tensile strength.

The calculation of effective bond density, particularly related to the PAT variable formation coefficient, FORM, is required to quantify sheet properties. If fibers are not uniformly distributed throughout the sheet, their network bonds will also not be uniformly distributed, resulting in areas of high and low bond density. Because the sheet tends to fail by a sequence of small failures at weak points, sheet strength is determined primarily by the strength at these weaker areas. By taking the product of the formation factor (a fraction between 0 and 1) and the bond density, the effective bond density can then be defined as a measure of the bond density of the weaker areas of the sheet.

SHEET ANISOTROPY

Sheet anisotropy (an-isotropic) is a term which describes the directional variability (MD, CD, $ ZD) of a formed sheet. A discussion of the factors used within MAPPS to quantify anisotropy follows.

Formation

Important aspect of sheet forming which introduces network anisotropy is formation. Formation relates to the spatial variation of the fiber mass distribution in the MD/CD plane and may be quantified as a variation in sheet basis weight and caliper, i.e., a variation in sheet density. Concepts used in modeling formation are illustrated in Figure 10.

The formation factor is determined by a combination of forming conditions and the stock characteristics (particularly fiber length and freeness). Fundamentally, formation is related to the formation and breakup of "flocks" in the turbulence fields of the flowing stock. However, modeling at this level is beyond the scope of the current status of MAPPS.

On a more practical level, the formation factor directly influences the properties of the sheet since poor formation leads to poor tensile properties as well as a poor visual appearance. For instance formation strongly contributes to the distinction between handsheets and machine-made paper. At the mill level, achieving good formation is a critical problem for high speed paper machines, while good formation is the norm on slow-speed machines and molds.

For research and process analysis applications, differences in formation between handsheets and machine paper make the prediction of machine paper properties from handsheet properties a difficult task. Thus a very important application for PATs is the direct prediction of machine paper quality. A key assumption of the PATs modeling system, then, is that formation not only affects the physical density distribution of the fibers but also the bond density. As noted earlier, for a perfectly formed dry sheet, the two are assumed to be identical.

In the PAT system, the impact of formation is modeled through the use of a parameter called the "formation coefficient," which has a value between 0 and 1 (1=ideal formation). The formation coefficient thus represents the coefficient of variation in density and, hence, the efficiency of bond formation since sheet density is proportional to bond density. Because the ultimate strength of the network is governed by the weakest members, the effective bond density is reduced as the formation coefficient drops below its ideal value of 1. Further, the effective bond density ultimately affects sheet strength through relative bonded area as described in later sections.

In summary, the five attributes modeled for the forming operation are the potential bonded areas of the top and bottom sides, the formation factor, the orientation ratio and the wet stretch factor. An overview of the bond development concepts is shown in Figure 8.

Surface Properties

Surface and printing properties depend on fiber characteristics and network bonding at or near the top and bottom surfaces of the sheet. The removal of most of the intrafiber moisture creates hydrogen bonds between the fibers which is assumed to lead to conversion of potential bonded area, Sb, to actual bonded area, Sa. Converting the network attributes for the potential bonded area of the top and bottom of the sheet (SB1 and SB2, respectively) by this theory linking fiber-fiber contacts to density results in differences in density from side-to-side and, thus, from surface to bulk.

By determining a surface bulk density and bond density for the top and bottom of the sheet ($\rho_b{}^t$ and $\rho_b{}^w$ respectively), surface properties such as Hunter gloss and roughness can be predicted for each side based on the bond density of that side. This concept is particularly important in studying the effects of calendering conditions on the sidedness of the sheet.

Sidedness and ZD variability also affect other sheet properties. Some of these effects are summarized in Table 1.

FIGURE 10 - CONCEPTS USED FOR MODELING OF FORMATION

- **Variability in BOND DENSITY is proportional to variation in SHEET DENSITY, ρ**

  i.e. $\Delta \rho_b \quad \Delta \rho$

- **The effective bond density, ρ_b^e, is based on the weakest link**

  i.e. $\rho_b^e = \rho_b - \Delta \rho_b$

- **$\Delta \rho_b$ increases with: consistency, fiber length, and high jet-to-wire speed ratio**

- **Tensile and elastic properties are affected**

FIGURE 11 - INFLUENCES OF SIDEDNESS

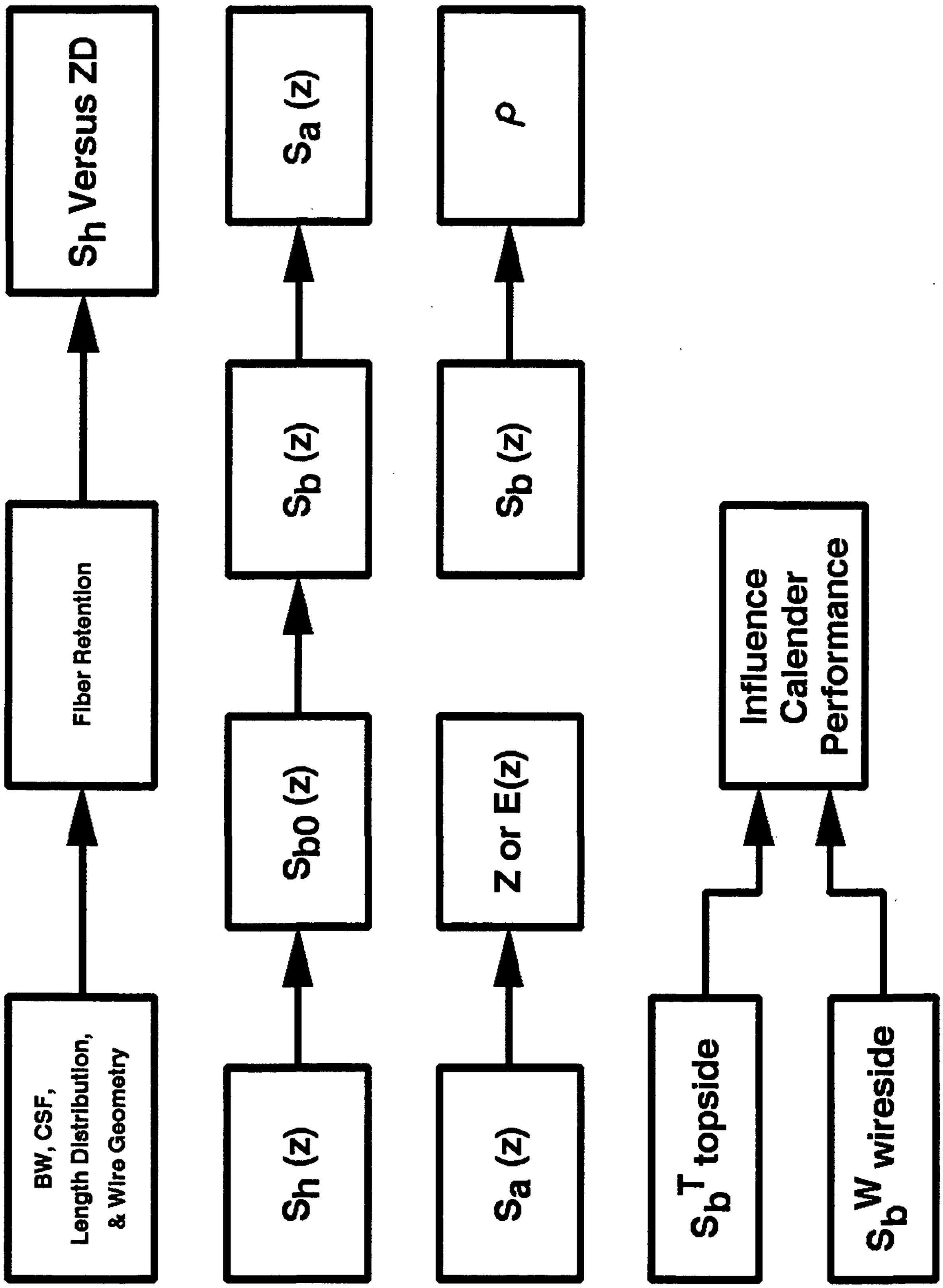


FIGURE 12 - OTHER BONDING EFFECTS

- **Repulping Dissolves the Network**

  network + water → slurry,   ASB → 0

- **Drying**

  Fibers collapse and stiffen
  Surface area decreases
  Stresses are "built-in" to the sheet

- **Calendering**

  Sheet is densified
  Bonds break depending on moisture & temperature
  Fibers collapse
  Under some high moisture conditions bonds may form

- **Refining, Mild Chemical Treatment**

  Restores fiber flexibility
  May reduce length, strength of fiber

TABLE 1 - EFFECTS OF SIDEDNESS AND ZD VARIABILITY ON SHEET PROPERTIES

Topside of Sheet	versus	Wireside of Sheet
Denser.............		Bulkier............
Smoother...........		Rougher............
Stronger...........		Weaker.............
More Bonded........		Less Bonded........
Lower Scattering...		Higher Scattering..

ZD Variability - Sidedness

The variability throughout the thickness of the sheet, referred to as ZD variability, is accounted for by the use of the fiber morphology and surface area attributes. As each layer of the sheet is formed, this information is stored in the ZD variability array where each row of the array contains attributes for each layer in the network. The influences of sidedness are illustrated in Figure 12.

TABLE 2 - INFLUENCES ON ZD VARIABILITY

- **ZD VARIABILITY is influenced by RETENTION**
- **RETENTION is influenced by:**

  Furnish
  - **Fiber Length**
  - **Freeness (specific surface)**

  Basis Weight Development
  - **Drainage Rate**
  - **Stock Consistency**

  Wire Geometry / Resistance

Some of the influences of fiber retention on ZD variability are summarized in Table 2.

Fiber Orientation

Fiber orientation is represented by a performance attribute parameter called the "fiber orientation ratio" (OR), defined as the cotangent of the average fiber orientation angle relative to the machine direction.

Anisotropy is also influenced by wet straining of the sheet near the end of the wire and in the dryer section. Like fiber orientation, stretch imparts preferential stress in the machine direction as represented by the performance attribute parameter "wet stretch" (WS). Together, the fiber orientation ratio and wet stretch influence the directional properties of the sheet. Thus many sheet properties are not isotropic (independent of direction) but vary in the three principal directions, MD, CD and ZD. The factors which influence directional properties are summarized in Table 3.

TABLE 3 - FACTORS INFLUENCING DIRECTIONAL PROPERTIES

■ **Fiber Orientation Ration**
■ **Wet Stretch**
■ **Bond Density**

ALTERATION OF THE SHEET STRUCTURE AND INTERFIBER BONDS

The sheet structure can be altered in a variety of ways during papermaking. Strength or retention aides can be added before the sheet is formed to alter fiber bonding or fines content. Fillers may also be added to increase opacity by occupying space between fibers and coatings may be applied to alter sheet surface properties. In addition multi-ply sheets may be formed to produce a composite structure with unique properties. At present these effects are beyond the scope of the PAT system but could be added at a later date.

In addition to the above-mentioned processes, sheet properties can be altered through converting operations. Calendering represents the most common and important converting process. Different calendering methods are used depending on the grade and forming method.

Ideally, the calendering operation is designed to remove sidedness and generate a smooth printable sheet surface without adversely affecting bonding, sheet strength, or reducing sheet bulk. Unfortunately, the application of pressure in the calender nip also decreases bulk and may cause fiber collapse and debonding due to shear stresses in the nip. However, unless moisture and temperature levels are high enough to soften the fibers and permit the formation of hydrogen bonds, the densification process usually does not lead to increased bond formation. The increase in fiber contact does tend to increase surface smoothness and by applying different treatments to each side, it is possible to reduce sidedness.

Within MAPPS, no new attributes are generated by the calendering operation. Instead, several key attributes such as actual and potential bonded areas are affected by moisture, temperature, and pressure which, in turn, affect sheet properties.

SHEET PROPERTIES

Handsheets

Given the PAT values of the fibers for a stream, the handsheet network is "assembled," i.e., formed to a specified formation, fiber orientation and strain, and pressed to a specified pressure, automatically in the MAPPS modules which calculate handsheet properties. Some modules are set up to predict properties of ideal handsheets, i.e., with ideal formation and random orientation, while others, such as PROPS and PROPS2, allow the user to specify the basis weight, formation, orientation, and stretch of the handsheet.

Machine Papers

Machine paper properties are based on the actual network PAT values, such as SB1, SB2, ASB, FORM, OR, and WS, as well as the usual fiber attributes. Thus, unless the sheet has been passed through a normal sequence of forming, pressing and drying operations, these attributes will not be present and no properties will be predicted for the machine paper.

Structural Properties

A wide variety of structural properties are computed by MAPPS, including sheet density, caliper and porosity. Sheet density is a function of top and bottom fiber contact areas (SB1 and SB2), cell-wall thickness (CWTH), yield, CSF, and fiber stiffness (SMOD) and in general, will increase with decreasing yield, thinner cell walls, lower wall stiffness, decreasing freeness, and increasing pressure. By a similar analysis, Gurley porosity increases with decreasing freeness and density and Caliper increases with increasing basis weight for a given density and decreases with density for a given basis weight.

Strength Properties

The sheet strength or breaking length model is based on a modified form of the Page Equation, in which the relative bonded area, RBA, is a function of the effective bond density, ρe, described earlier. Thus, RBA accounts for not only species, pulping, bleaching, and refining but also for forming and pressing and other effects as well. The other variables in this sheet strength model include the intrinsic fiber tensile strength, FTENS, the specific bond strength, SBSTR, the average fiber length, AVGL, and the average fiber width, AVGW.

In general, MD tensile strength will be more dependent on bonding than on the intrinsic fiber tensile strength. Thus, the MD tensile strength will be more sensitive to either RBA or bond strength. Because RBA tends to reflect sheet density and formation, low strength can occur because of low sheet densification or poor formation as well as poor bond strength. MAPPS currently does not have a way of predicting specific bond strength. This PAT variable is initialized in the WOOD02 module through the species database and can readily be overwritten with a user-specified value in this module or adjusted in a GENPRS block to adjust the overall level of strength. The concepts involved in modeling strength are shown in Figure 13.

FIGURE 13 - TENSILE STRENGTH MODEL

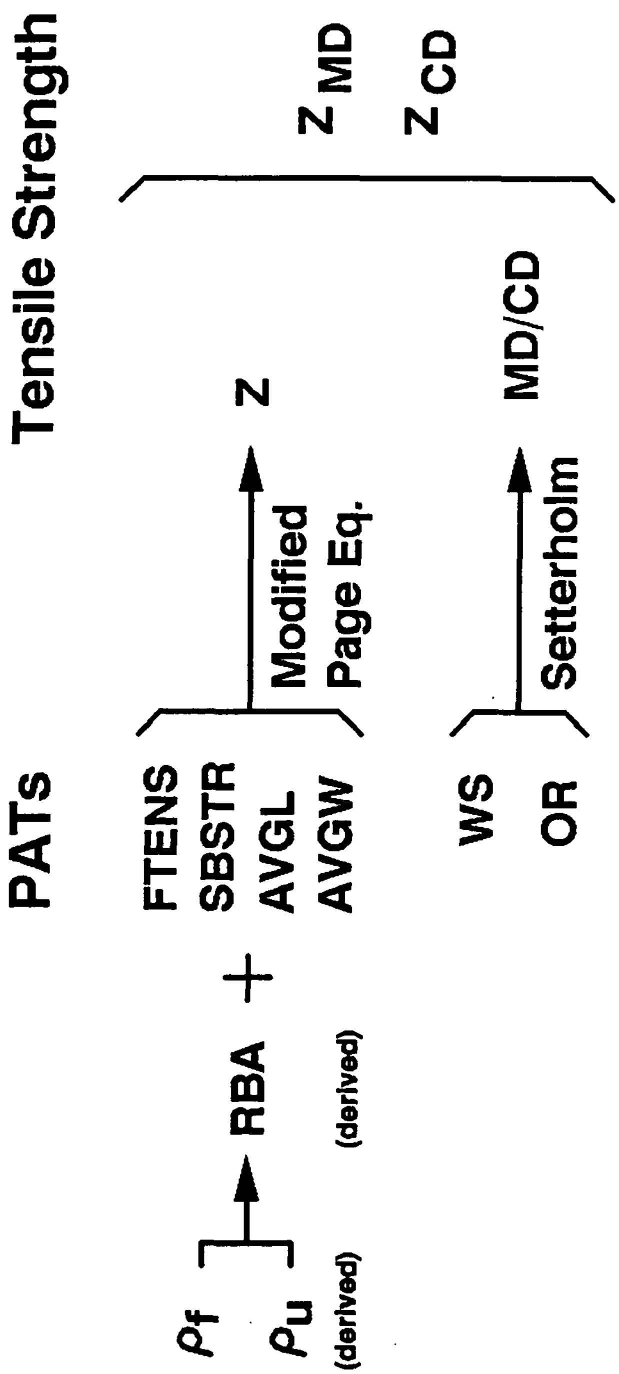
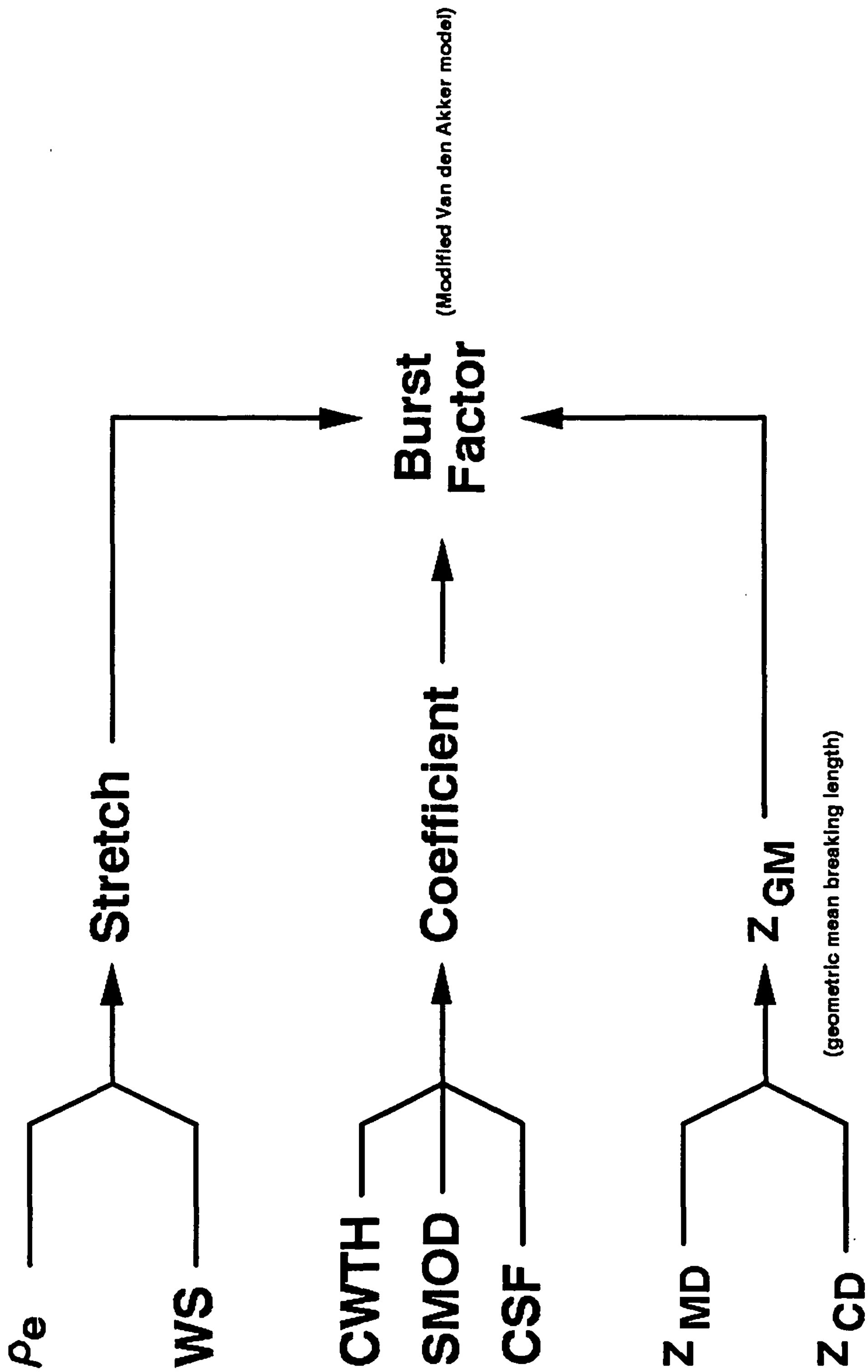


FIGURE 14 - BURST FACTOR MODEL



MD/CD tensile ratio is a function of fiber orientation ratio, OR, and overall sheet strain, WS, during formation and pressing, due to speed differentials along the machine. As OR increases above 1 and WS increases above 0, MD/CD ratio tends to increase above 1. Given typical values of OR = 1.5, and WS = 1%, the resulting, computed MD/CD ratio would be 2.2. The MD tensile tends to increase above its geometric mean as the square root of MD/CD ratio and the CD tensile decreases to maintain the ratio.

Elongation at break is a linear function of effective bond density and wet strain. Thus, as the sheet becomes stronger, stretch decreases. Similarly, as the overall strain on the sheet increases, stretch at break decreases. Bulkier and weaker sheets tend to strain more before failure.

Burst Factor

The burst factor model is based on a slightly modified version of the Van den Akker model and is primarily a function of the geometric mean breaking length and the square root of the elongation at break, (stretch). Thus, as the strength increases, the burst factor tends to increase. However, as the stretch of the sheet, WS, increases, elongation at break tends to decrease while geometric mean strength remains constant, reducing the burst strength. The basic theoretical model is modified with a coefficient which depends on cell-wall thickness (CWTH), CSF and fiber stiffness (SMOD), as shown in Figure 14.

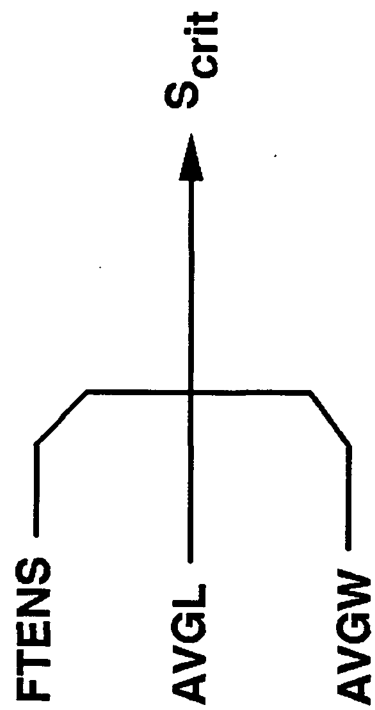
Elastic Properties

Elastic properties are based on data by Fleishmann and Bernard Berger. The elastic stiffnesses, Ex, Ey, and Ez, and the shear and compressive stiffnesses, Gxy, Cx, Cy, Cz, are functions of effective bond density (ρe), fiber modulus (FMODU), fiber orientation (OR) and strain (WS). The concept is illustrated in Figure 16. In general, as sheet density increases and formation improves, sheet stiffnesses tend to increase, at least in the MD/CD plane. As fiber orientation and strain increase, and the MD/CD ratio increases, Ex increases and Ey decreases.

Tear Strength

Tear strength is based on a model by Shallhorn and Karnis. As shown in Figure 15 the average fiber length and width (AVGL and AVGW) and fiber tensile strength (FTENS), determine a critical shear stress, SCRIT. If the calculated critical shear stress is smaller than the PAT variable SBSTR (specific bond strength), the tear factor is calculated based on a model which depends on the effective bond density (ρe), AVGL, AVGW, CWTH, and specific bond strength (SBSTR). If the calculated critical shear stress is greater than SBSTR, the tear factor is calculated by another model which includes fiber tensile strength (FTENS), as well as the other variables.

FIGURE 15 - MODIFIED SHALLHORN & KARNIS TEAR FACTOR MODEL



If S_{crit} < SBSTR → Tear Factor Model 1

$TF_1 = f(\rho_e, AVGL, AVGW, CWTH, SBSTR)$

If S_{crit} > SBSTR → Tear Factor Model 2

$TF_2 = f(\rho_e, AVGL, AVGW, CWTH, SBSTR, FTENS)$

FIGURE 16 - MODEL FOR ELASTIC PROPERTIES

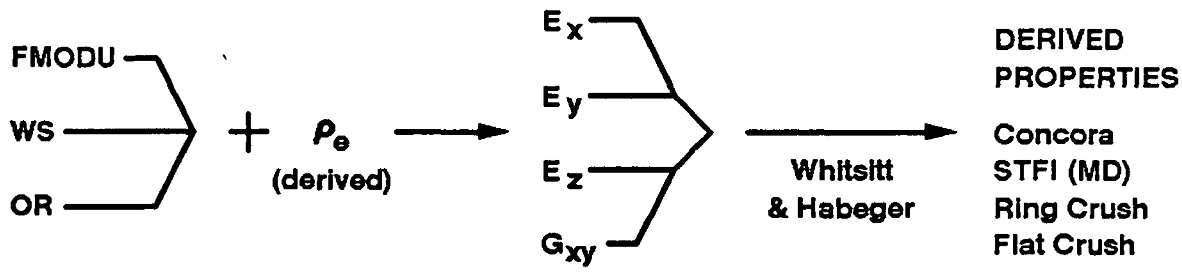
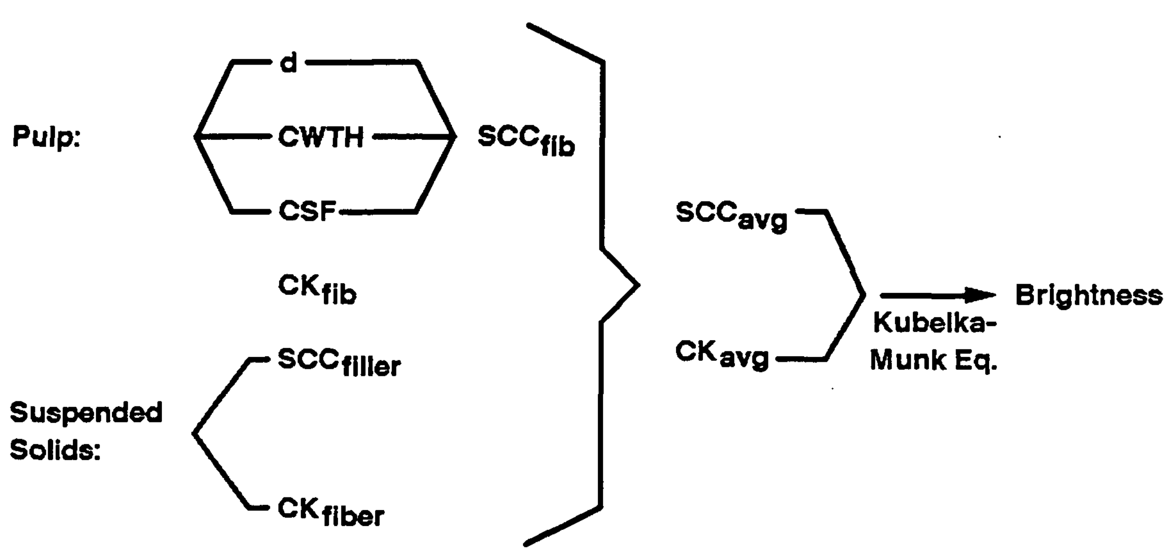


FIGURE 17 - OPTICAL PROPERTIES MODEL



Compressive Properties

A variety of compressive properties are modeled in the system. Properties include compressive moduli, C_x, C_y, and C_z, which are functions of E_x, E_y, and E_z, based on work of Habeger and Whitsitt. Failure compressive properties derived from these include MD STFI, CD ring crush, flat crush, and concora. MD STFI and CD ring crush are functions of E_x and E_y or E_y and E_z, respectively. Flat crush is then derived from STFI and concora is derived from flat crush. These latter properties are actually functions of E_{xt}, E_{yt}, and E_{zt} as well as the sheet caliper. Thus, these properties are functions, not only of fiber modulus and bond density but also of basis weight.

Surface Properties

As mentioned earlier, surface properties, such as roughness and gloss, are modeled as functions of surface density. Surface density is determined from SB1 and SB2 for each surface and the compressibility of each surface. Generally, surface compressibility will increase with increasing CSF, increasing CWTH, and increasing yield. However, the surface density will be the lowest when the fiber conformibility is the highest, which tends to be when CSF is low, yield is low, and cell walls are thin, i.e., CWTH is low. This apparent contradiction arises from the fact that high fiber conformibility results in rapid sheet densification and low compressibility, while stiff fibers which do not readily conform result in high compressibility but, generally, lower density.

Optical Properties

Surface light scattering is modeled in terms of contact areas which are assumed to be proportional to sheet density. Other factors are the number of reflecting particles, which is related to CSF and to the loading of fillers. As shown in Figure 17, the fiber contribution to the scattering coefficient, SCC, depends on sheet density (d), cell-wall thickness (CWTH) and freeness (CSF). If suspended solids are present, the mixture SCC is calculated as the weighted average of the scattering coefficients of the fibers and the fillers. The filler SCC is a function of the weighted average of any suspended material added during the process.

The absorption coefficient, CK, of the fibers and fillers also contributes to brightness. If any fillers are present, the mixture CK is calculated as the weighted average of the absorption coefficients of fillers and fibers. Brightness is then computed from the Kubelka-Munk equation using the mixture scattering and absorption coefficients.

The effect of dyes must currently be simulated by manually increasing the absorption coefficient of the fibers based on the type and loading of dyes. However, an automatic calculation procedure based on spectral color is now being tested and will be available at a later date.

OVERVIEW OF UNIT OPERATIONS

Most of the mass and energy transport inherent in papermaking alter one or more performance attributes. Conversely, the mass and energy performance of an operation may also be influenced by a performance attribute parameter. Table 4 summarizes the unit operations which work with performance attributes.

Performance attributes are changed in an input-output mode as shown in Figure 18. Thus, it is possible to track the development of various performance attributes since each material stream also has a parallel performance attribute stream.

The MAPPS module PROPS can then be used to calculate a set of end-use paper properties typically measured in a paper mill's product testing laboratory. The PROPS module calculates these end-use properties based on the input of a material stream and the corresponding performance attribute stream. The development of paper properties throughout a process can thus be tracked by inserting several PROPS modules at different locations in the simulation.

TABLE 4 - SOME UNIT OPERATIONS INVOLVING PAT MODELING

SPECIES
Initial "intrinsic" properties of wood..
PULPING
Chemical, mechanical....................
BLEACHING
REFINING
MIXING
SEPARATIONS
Screening................................
Cleaning (hydrocyclones)................
Decker operation........................
SHEET CONSOLIDATION
Forming..................................
Wet Pressing............................
Drying...................................
CONVERTING
Calendering.............................

Wood Species

The MAPPS module WOOD02 can be used to initialize a material stream of the pulping, bleaching, or paper type (stream types 3, 5, or 6). The user initializes the flows of chemical components by specifying a set of module parameters. The user can then initialize the performance attribute parameters for the material stream by specifying them individually or by specifying the species the flow is meant to represent.

MAPPS has a species data base which contains data for wood fibers from 19 different species. When specifying a species in the WOOD02 module, MAPPS will access this species data base and assign default values for all performance attributes which are not specified by the user. It should be noted, however, that the data in the species data base is only valid for unpulped, unrefined wood fibers (i.e. wood chips). Thus, if the WOOD02 module is used to initialize a material stream representing a bleached pulp flow, for example, the species data base default values for various performance attributes may not be correct.

Chemical Pulping

The primary purpose of pulping is to break down the wood chips into fiber bundles, and then to individual fibers. In chemical pulping, this objective is met by chemically dissolving the lignin, the component holding the individual fibers together in the wood structure and, simultaneously dissolving most of the hemicelluloses and a small fraction of the alpha-cellulose. Dissolution of lignin and cellulose takes place in the digester and fiber separation typically takes place when the pulp is blown from the digester to the blow tank. For higher yield pulps, a low consistency refiner following the discharge may be required to obtain the desired fiber separation.

The pulp yield for a chemical pulp is typically in the 40-60% range, i.e., about half of the original wood material is lost. Chemical pulping results in fibers that are more pliable, wettable, and have a higher bonding potential than fibers from a mechanical pulping process. Chemical pulping reduces the value of the performance attribute parameters yield, kappa number, and hemicellulose-to-cellulose ratio and changes in these attributes affect sheet consolidation and other operations downstream. In a mill, the yield loss is partially compensated for through energy recovered by burning the black liquor from the pulping operation and the simultaneous generation of a significant portion of the energy requirements of the process. However, the recovery process does not contribute to the PAT modeling feature of MAPPS.

High-Yield Pulping

Mechanical pulping (high-yield) relies on combinations of mechanical action (refining or grinding), heat, and some mild chemical pretreatments to separate fibers with very little yield loss. The result is a distribution of fibers, fines, and shives (bundles of unseparated fibers). Mechanical pulping generates a pulp with more hydrodynamic specific surface area and a corresponding lower freeness than chemical pulping. However, the higher lignin content results in stiffer fibers which do not bond as effectively as the more pliable fibers of chemical pulp. Thus, while there is more area to bond, the bonding efficiency is lower for mechanical pulps. Chemical pretreatment used in conjunction with mechanical pulping, removes some lignin, generates less stiff fibers, and shifts the bonding behavior toward that of chemical pulps.

FIGURE 18 - PROPS MODULES TRACK PAPER PROPERTY DEVELOPMENT

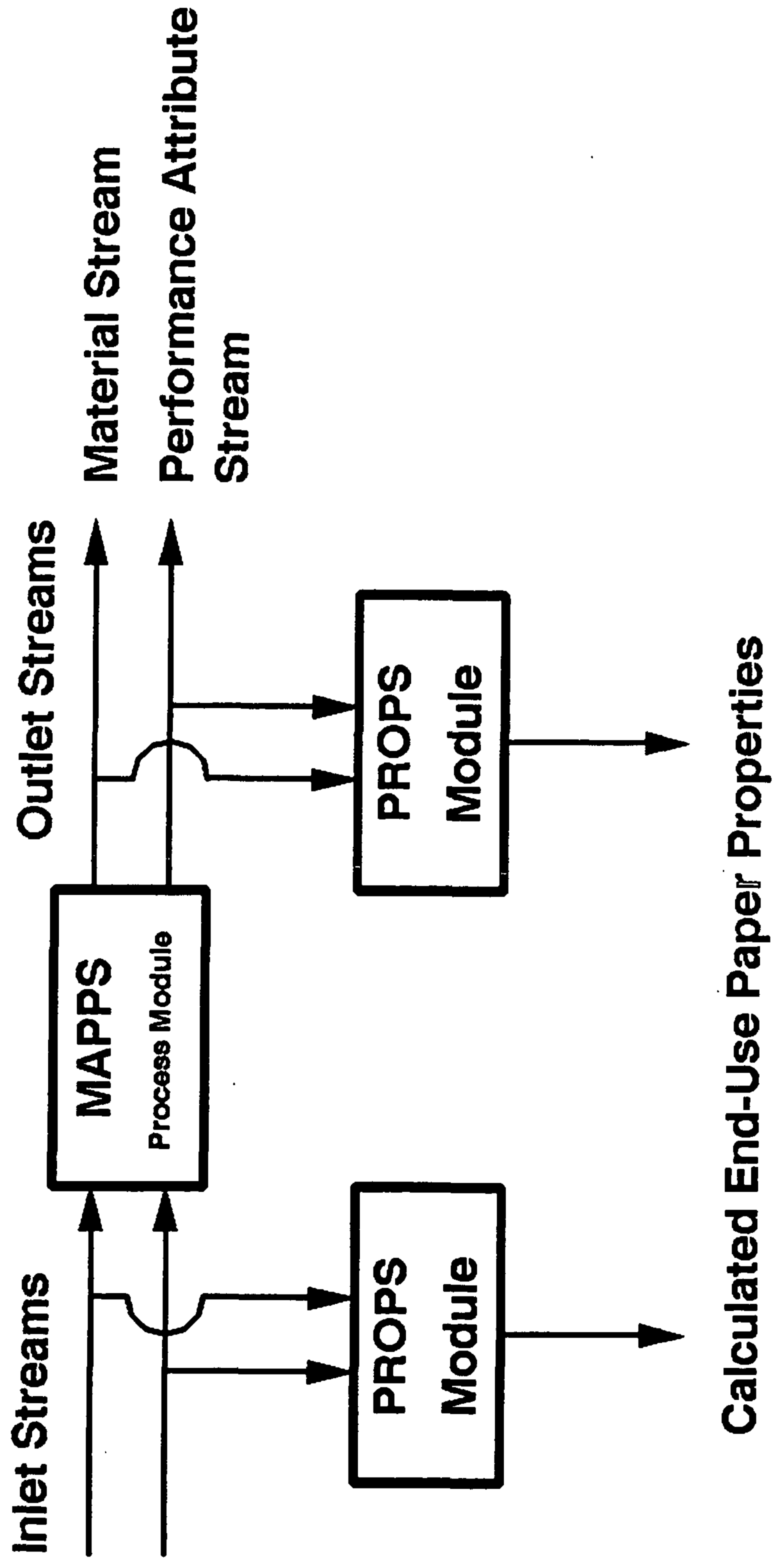
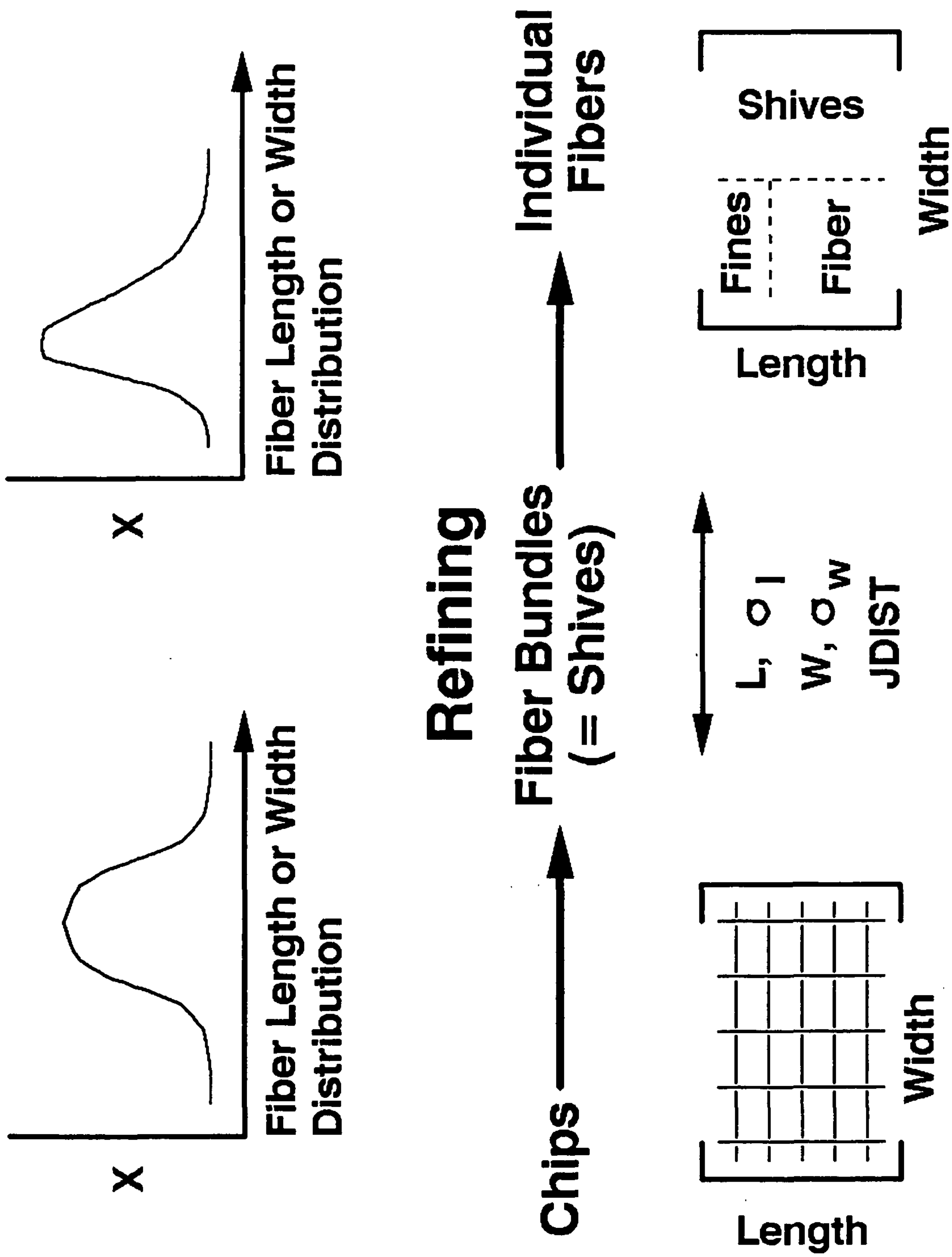


FIGURE 19 - TRACKING OF CHANGES IN FIBER MORPHOLOGY



Refining of pulps also increases the intrinsic strength of fibers by opening up the internal structure. MAPPS simulates this effect by increasing by the fiber tensile strength in relationship to the surface area developed during refining. Some advantages of using performance attribute modelling to simulate refining are shown in Table 5 which compares the performance attribute modelling features for refining with those of conventional simulation. Conceptually, the PAT system can be used to track changes in fiber morphology and surface area in pulping, refining, screening, and cleaning operations, as shown in Figure 19.

A unique advantage of performance attribute modelling is that it allows a dual representation of a fibrous material stream. Through various performance attribute parameters, a stream can be represented both in terms of its chemical components: cellulose, hemicellulose, and lignin, and in terms of its fiber fractions: fiber types 1-9, shive types 1-3, and fines, as illustrated in Table 6. PAT information provides the means to convert from one stream type to another (for example, from a pulping type stream to a paper type stream), while preserving the effects of processing conditions on the fibers.

TABLE 5 - ADVANTAGES OF USING PATS FOR MODELLING OF REFINING

CONVENTIONAL SIMULATION	CONVENTIONAL SIMULATION PLUS PERFORMANCE ATTRIBUTES
Arbitrary fiber conversion specified by user...........	Fiber length and width distributions are calculated
Energy consumption..........	Meaningful representation of fines, fibers, shives.......
	Surface area development....
	Change in intrinsic fiber strength....................

TABLE 6 - DUAL REPRESENTATION OF FIBERS

PERFORMANCE ATTRIBUTE PARAMETERS:	MATERIAL FLOW PARAMETERS:
Kappa Number....................	Chemical Composition of Flow:
Hemicellulose Ratio............	Cellulose..................
	Lignin.....................
Fiber Length Distribution......	Flow Composition in Fiber Categories:
Standard Deviation of Length...	Fiber Types 1-9............
Fiber Width Distribution.......	Shive Types 1-3............
Standard Deviation of Width....	
Distribution Type..............	Fines......................

Screening and Cleaning

Screening and cleaning operations are designed to remove unwanted material such as shives and debris from the pulp prior to sheet forming. Screening separates longer fibers and shives from shorter fibers resulting in accepts flows (or overflows) which tend to have a lower shives content and a shorter average fiber length than the reject flows (or underflows). Hydrocyclone cleaners separate fibers based on fiber surface area or density. Thus, dirt and heavy debris generally leave with the rejects, while fibrous materials, which have a high surface area and a high L/D ratio (length-to-diameter ratio), and other less dense material leave with the accepts.

The stock leaving a screening and cleaning system will have a lower shives content, higher fines content, lower average length and width, higher specific surface area, lower freeness, and higher bonding potential area than the entering stock flow. Thus, the performance characteristics of the screening and cleaning operations are strongly dependent on the performance attribute parameters for the fibers.

Screening and cleaning tend to accentuate differences between performance attributes. To utilize the equipment performance prediction features of MAPPS screening & cleaning modules, the user must specify equipment characteristics such as screen slot size, pressure drop, etc. Using the appropriate PATs, MAPPS then calculates the physical flows and attributes of the accept and reject streams.

Figures 20 and 21 illustrate differences between screening and cleaning and their effects on performance attribute parameters and end-use paper properties.

Mixing

Mixing of various stocks occurs frequently throughout the pulping and papermaking process. The PAT system mixes fiber attributes as well as material and energy. Most performance attribute parameters are mixed based on relative mass flows.

Some mixing operations involve reslurrying of the wet or dry sheet. Since reslurrying involves a dissolution of the fiber network, performance attribute parameters which represent the network are changed.

MAPPS modules which simulate screening, cleaning, refining, and stockmixing, calculate handsheet properties based on the fiber composition and performance attributes of the streams entering and leaving each module, providing information needed for a detailed analysis of the stock prep system for optimal design and reduced energy consumption.

FIGURE 20 - STOCK CLEANING OPERATION

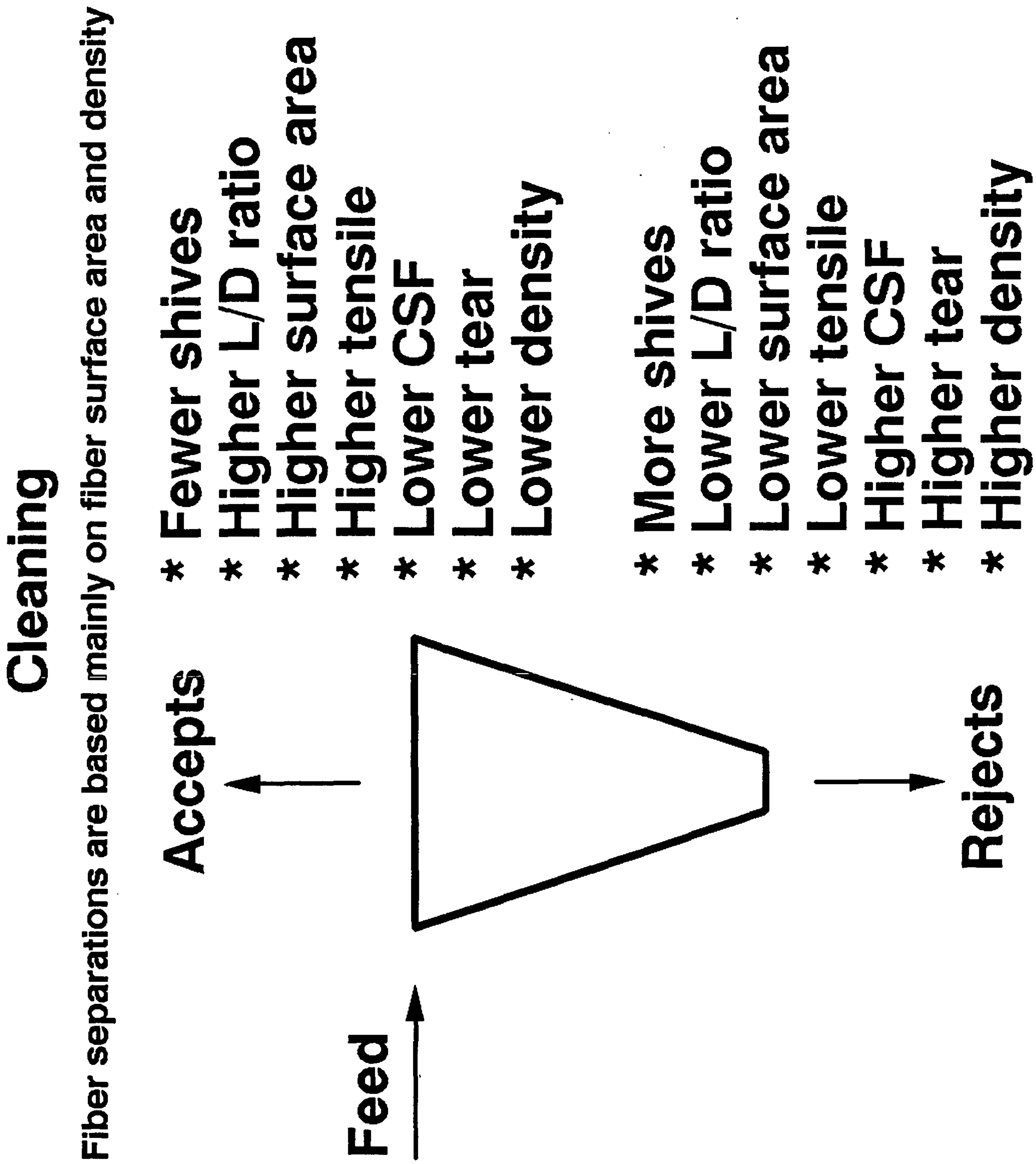
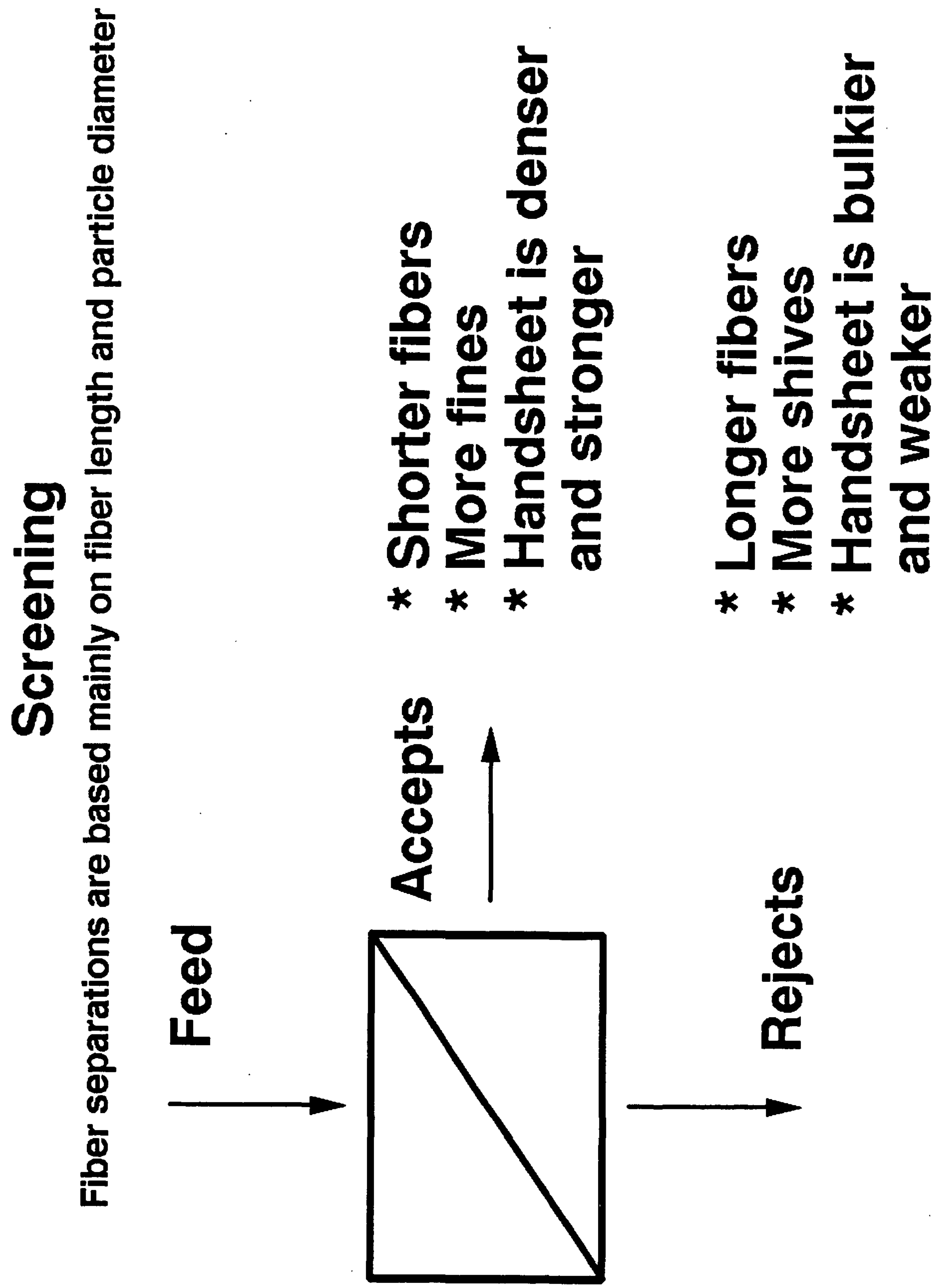


FIGURE 21 - STOCK SCREENING OPERATION



Sheet Forming

In papermaking operations, the sheet is formed as the stock impinges on a wire which moves at approximately the same speed as that of the stock from the headbox. The stock is a dilute slurry of mainly fibers and fillers or other additives. The fibers are deposited on the wire by a filtration mechanism rather than a thickening mechanism. For this reason, a rather dense layer of fibers forms on the wire, leaving the fiber slurry above the formed mat at a relatively constant consistency. The white water which drains from the slurry contains fines and suspended material and generally is at a lower consistency than the slurry.

As the fiber mat forms on the wire, the mat basis weight (mass/area) increases so that more of the fine material in the slurry is retained by the mat thus decreasing white water consistency. Beyond the initial gravity drainage zone, drainage is assisted by the application of vacuum through various devices, like foils and vacuum boxes placed underneath the wire.

The PAT system accounts for many aspects of the forming process, including retention, wire and drainage element design and location. The model includes various filtration resistance functions which account for local turbulence level, sheet basis weight, pulp freeness, and other factors and as mentioned above, accounts for formation effects, fiber orientation, stretch, and Z-D variability in fiber distribution and surface area.

Table 7 below illustrates some of the advantages of using performance attribute simulation to model sheet forming.

TABLE 7 - ADVANTAGES OF USING PATS FOR MODELING SHEET FORMING

CONVENTIONAL SIMULATION	CONVENTIONAL SIMULATION PLUS PERFORMANCE ATTRIBUTES
Modeled with mixers and splitters...................	Detailed dewatering and drainage.....................
NonPredicted...............	Design details included.....
	PATs influence dewatering retention and formation.....
	Sheet Anisotropy............
	Sidedness...................
	More Predictive.............

The sheet forming module also includes submodels of individual drainage elements, a dandy roll, and the headbox giving the user the ability to model forming with one block or, alternatively, with a series of forming blocks. In addition to a fourdrinier model, there is a multi-ply forming model which determines similar characteristics for a variety of multi-ply forming configurations.

Sheet Consolidation and Wet Pressing

The wet pressing model determines the degree of dewatering and sheet consolidation that occurs in a single press nip and computes the press power requirements. Required information includes felt basis weight, sheet basis weight, machine speed, entering moisture content, press speed, and lineal nip loading.

Table 8 below, compares some of the advantages of using performance attribute simulation to simulate dewatering over conventional approaches.

TABLE 8 - ADVANTAGES OF USING PATS FOR MODELING OF PRESSING

CONVENTIONAL SIMULATION	CONVENTIONAL SIMULATION PLUS PERFORMANCE ATTRIBUTES
Water removal based on stream splitting only.......	Dewatering depends on: furnish characteristics... press design.............. press conditions.......... Sheet consolidation......... Z-D variability simulated... Power consumption.........,.

The mass and energy portion of the model uses the incoming mass and energy flows and PAT information, particularly freeness, to compute nip residence time, maximum nip pressure, dewatering time constant, and moisture removal. The performance attribute portion of the model computes the sheet compressibility and the increase in potential bonded area resulting from pressing.

Drying

MAPPS contains a fairly detailed and reliable mass and energy balance model of the dryer section of a paper machine. The PAT system adds submodels for several performance attribute parameters based on the amount of moisture removed during drying. These effects were discussed in an earlier section on sheet bonding.

Table 9 compares conventional simulation with conventional simulation enhanced with performance attribute simulation in the area of drying.

TABLE 9 - ADVANTAGES OF USING PATS FOR MODELING OF DRYING

CONVENTIONAL SIMULATION	CONVENTIONAL SIMULATION PLUS PERFORMANCE ATTRIBUTES
Steam & air consumption.....	Steam & ari Consumption.....
Water removal...............	Water removal...............
	Bond formation..............
	Sheet consolidation.........
	Fiber stiffening............
	Fibrillar collapse..........

Calendering

Although calendering is not a major consumer of energy, its effect on final sheet properties is significant. The calendering model consists of several submodels which compute densification, heat transfer, and changes in paper properties taking place as a result of calendering. The heat transfer submodel determines heat exchange between the sheet and the roll in the nip and over the roll surface.

Sheet densification is a function of nip loading (lineal nip pressure), speed differential between sheet and roll, sheet temperature, and sheet moisture. Debonding of the network may also occur, based on the sheet moisture and temperature of the sheet and degree of densification in the nip.

TABLE 10 - MAIN FEATURES OF THE CALENDERING MODEL

Sheet is densified..
Property development differs on each side....................
Heat Transfer computed:
Nips...
Roll surface...
Two wrap configurations considered...........................
Thermal softening influences property development...............
Bonding or debonding may occur depending on moisture & temp.....
Calendering Application
Conventional...
Supercalendering.....................................
Gloss calendering....................................

Each side of the sheet may be affected differently if there is Z-D variability in the network attributes. Important printing properties such as gloss and surface roughness are computed in addition to tensile properties which will be affected by the degree of bonding or debonding that occurs in the nip. Using this spectrum of effects various types of calendering may be simulated.

Table 10 summarizes the main features of the calender model, showing how essential PATs are to property development.

Bleaching

The main purpose of bleaching is to dissolve color bodies located mainly in the residual lignin in the pulp. By removing these light-absorbing bodies, the fibers are brightened thus reducing the light absorption coefficient. Dissolution of the color bodies usually results in removal of much of the residual lignin, reducing the kappa number.

Severe bleaching conditions and bleaching with oxygen can also oxidize some cellulose or hemicellulose resulting in a reduction in yield, while bleaching with hydrogen peroxide dissolves color bodies without actual removal of lignin. Peroxide is widely used with high-yield pulps to brighten while preserving yield.

Another important result of bleaching is a softening of the fibers, primarily as a result of lignin removal. The softening is probably most pronounced for previously dried fibers. Therefore, the fiber stiffness factor is reduced to a value of one in any bleaching stage restoring the fiber to a natural predried stiffness.

MAPPS has a number of modules which handle a wide variety of bleaching processes. There are modules for bleaching with chlorine, chlorine dioxide, hydrogen peroxide, oxygen, and alkaline extraction with or without oxygen addition, and, in addition, a generic bleaching module is available to handle any other bleaching operations.

Property Utility Blocks

The PATS system contains many other important modules which perform a variety of functions. Perhaps the most important of these are PROPS and PROPS2, modules which compute a number of handsheet and machine-made paper properties at any location in the process, for single-ply and multi-ply sheets, respectively.

OTHER UNIT OPERATIONS

MAPPS contains many other modules whose main purpose is computation of mass and energy balances. Many of these are in the areas of chemical recovery, and steam and power systems are essential for a complete simulation and prediction of energy impacts.

SHEET PROPERTIES

There are hundreds of important sheet properties or specifications which depend on the grade and end-use of the product. A few important properties computed by the system are discussed below. Properties can be divided into general categories such as physical properties, tensile properties, surface or printing properties, and optical properties. Tensile properties can be subdivided into destructive and nondestructive.

Table 11 shows the factors which affect properties for the two main categories of sheets, handsheets and machine papers. The property models are the same for both types of paper. However, factors which are important for one type may not be important for the other. For example, formation usually differs significantly between handsheets and machine paper.

TABLE 11 - PAT SYSTEM RECOGNIZES TWO TYPES OF SHEETS

Two Types of Paper
Handsheets..
Machine Papers..
Major Factors Resulting in Differences Between Handsheets and Machine Papers:
Wet Pressure..
Fiber Orientation.......................................
Wet Stretch...
Formation...
Sidedness...

Table 12 summarizes the main property categories for which models are available.

Sheet density, which influences most other properties, should be considered as a primary property. As mentioned earlier, sheet density is strongly related to the fiber optical contact and to potential bonded area. In most situations were fiber bonding potential occurs, sheet density is an excellent measure of inter-fiber bond density.

Since network strength is related to a combination of fiber strength and bond strength, sheet density is usually a controlling variable, except at very high degrees of bonding where fiber tensile controls.

However, there are several situations in which fibers are brought closer together and yet the strength is low. For this reason, the PAT system defines a separate attribute for actual bonded area, which influences strength and potential bonded area, which influences sheet density and certain optical properties. The two are linked in the drying step, where hydrogen bonds are formed in the presence of moisture and temperature and in the calendering step where high densification conditions may destroy bonds, especially when calendering at low temperature and moisture.

FIGURE 22 - SHEET DENSITY VARIATIONS DUE TO WET PRESSING & REFINING

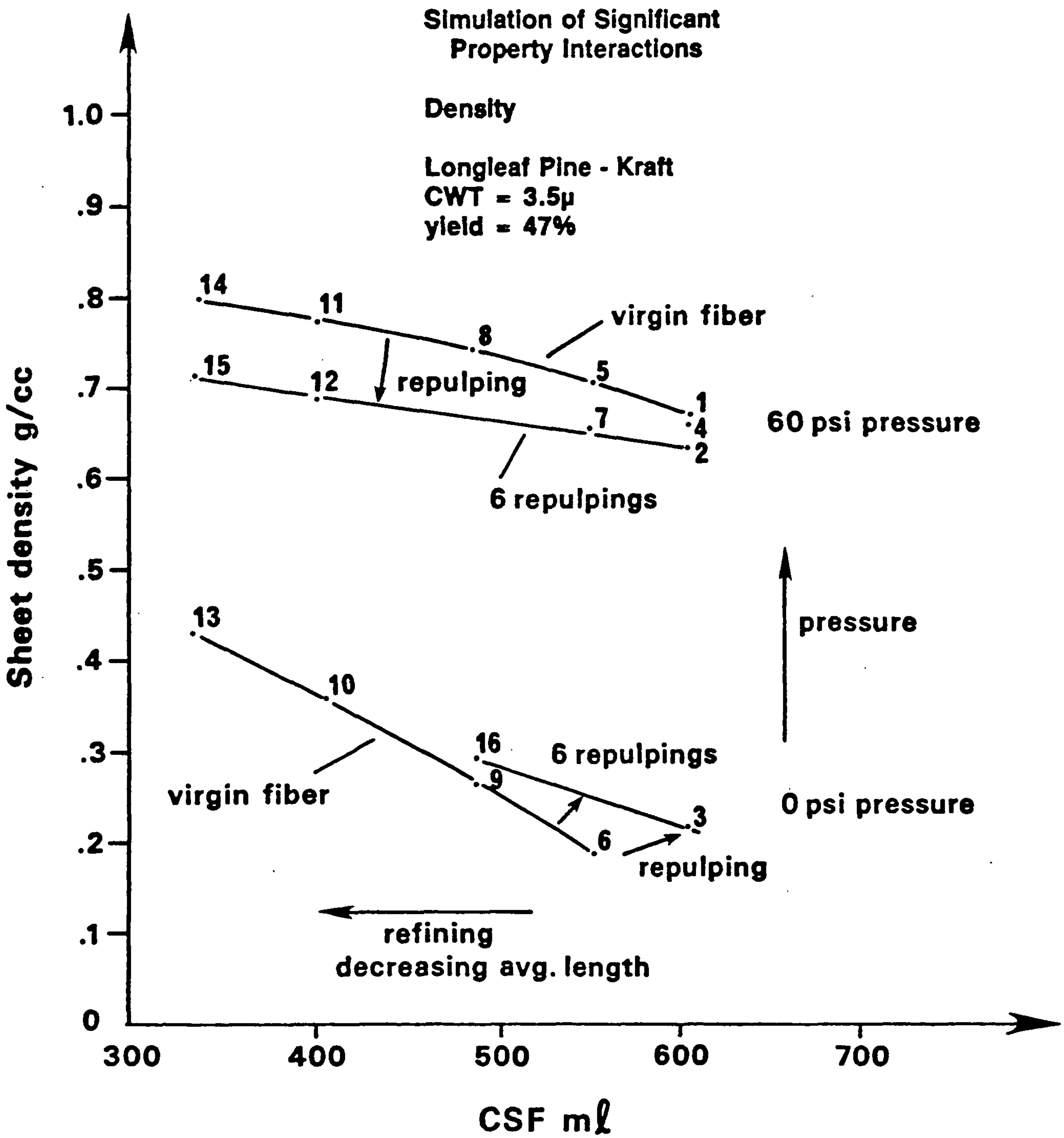


FIGURE 23 - BURST FACTOR AS A FUNCTION OF SHEET DENSITY

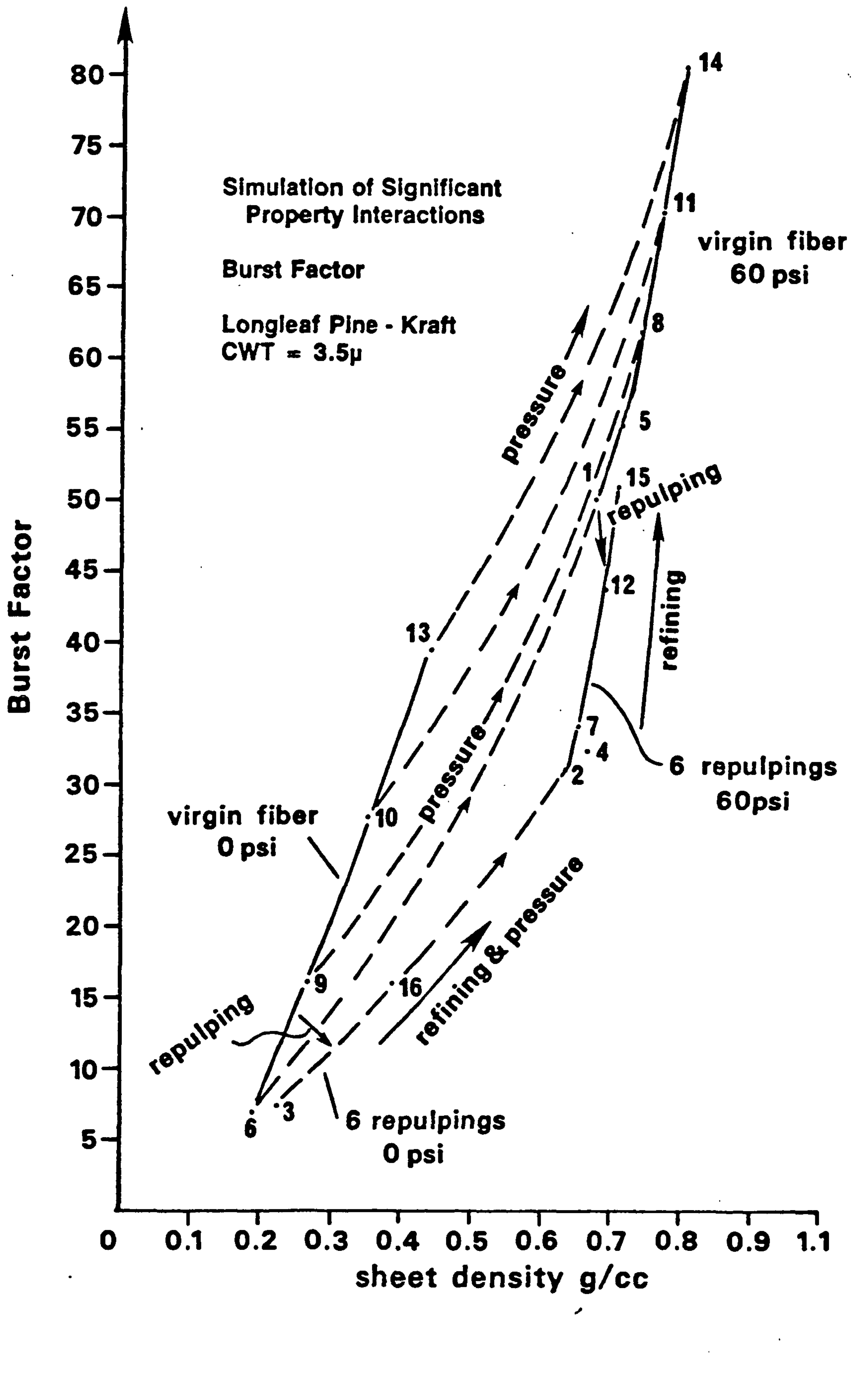


FIGURE 24 - TEAR FACTOR AS A FUNCTION OF SHEET DENSITY

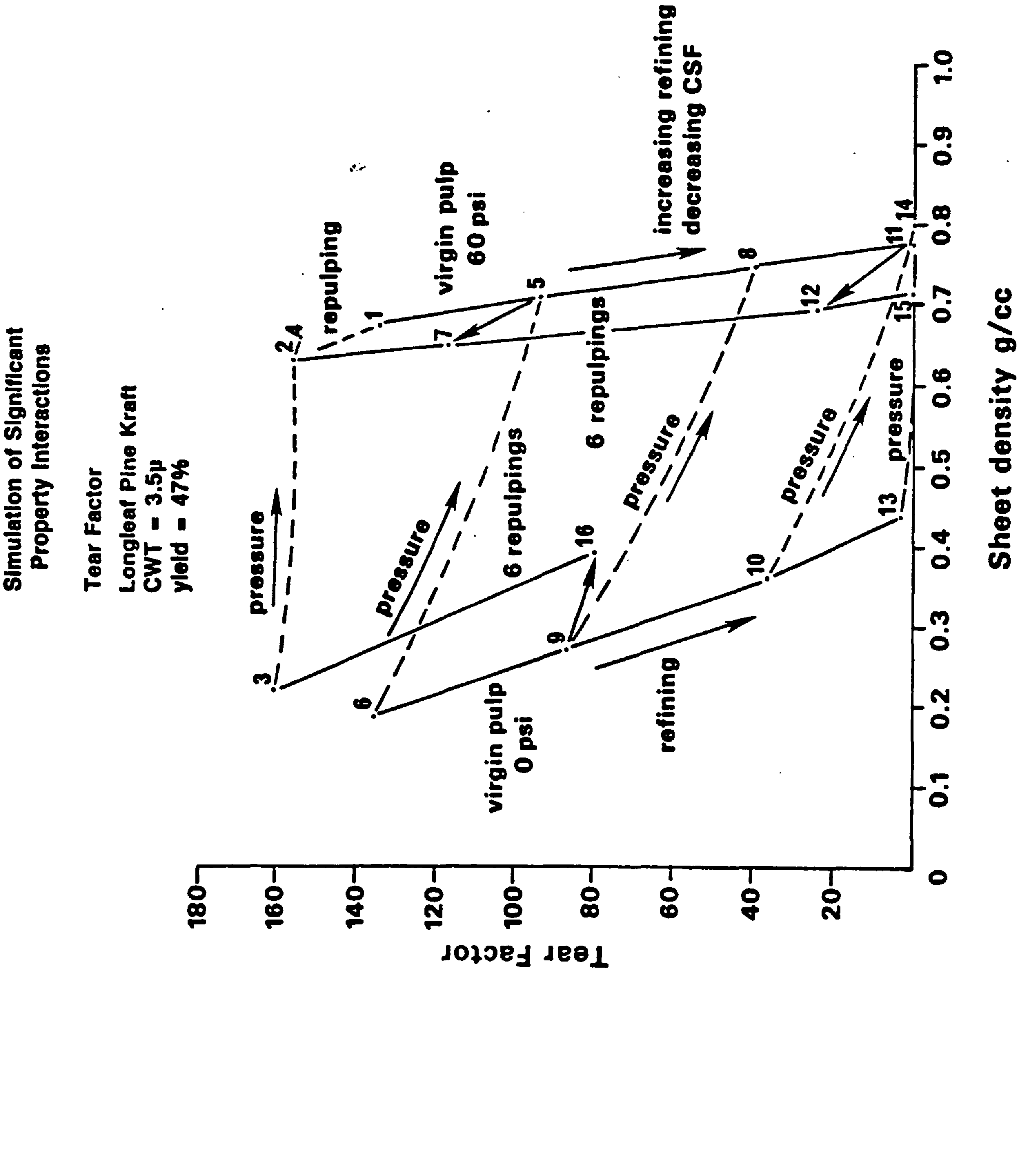


TABLE 12 - MAIN PROPERTY CATEGORIES

Structural...............	Density............... Porosity..............
Non-Destructive...........	Young's Modulus....... Directional Moduli....
Destructive..............	Directional Tensile... Compressive Strength.. Breaking Length....... Stretch............... Burst, Tear, TEA......
Surface Optical Printing..	Scattering............ Brightness............ Opacity............... Smoothness/Roughness..

Conversely, high moisture conditions also weaken bonds, and can result in strength loss without significant reduction in sheet density. Ultimately, when enough moisture is added to the sheet, the network breaks up and all strength is lost. For this situation the actual bonded area is reduced to zero and the potential bonded area is reduced as appropriate.

In addition, there is some loss of external surface area and some stiffening of the fibers in the drying step reducing the bondability of the fibers and, thus, the sheet forming characteristics of repulped fibers.

APPLICATIONS

The PAT system has been used to develope a wide variety of mill simulation models (2-7). Examples include TMP, CTMP, Medium, Liner, Fine Papers, Kraft, Groundwood, and Recycle Operations. While it is not feasible to discuss the effects of all of the combinations of process and property models for these operations, several applications are briefly discussed below. Please refer to the Module Technical Guide and the Programmer's Guide for a more in-depth discussion of the available property modules.

Three important properties, density, burst and tear, as shown in Figures 25 through 27, have been selected to illustrate the interactions of process conditions and property development.

As shown by Figure 25 sheet density generally increases with wet pressing pressure and refining (decreasing CSF). However, the response to either refining or pressing is different as both conditions are varied simultaneously. The effects of multiple repulping can be seen by comparing the lines marked "virgin fiber" (zero repulping) with the lines marked "six repulpings." Repulping, which tends to stiffen fibers, reduces sheet density at normal pressing pressures of 60 psi but there is a small increase at zero pressing pressure and low refining levels (500-600 CSF).

The effects of repulping are similar to those that can be seen between fibers of different wall thicknesses. Thus, a comparision of virgin fiber and fiber which have gone through six repulpings mimics the differences between or within species of different fiber wall thickness. Although not shown in the figures, increasing yield from 47% to 100% shifts the response curves downward, increasing the response to pressure and freeness.

Figure 26 shows the response of burst factor to density at various levels of pressure and repulping. Increased refining and pressure generally result in an increase in burst but the burst factor response to each varies with the other. Repulping tends to reduce burst, as it does with most tensile properties. However, the effects of repulping on burst can be partially overcome by refining and pressing.

Figure 27 shows the dependence of tear factor on sheet density which in general, changes in direction opposite to burst factor. The different response can be partially explained by the fact that tear is more dependent on fiber length than either density or burst. Thus, as refining increases, fiber length decreases to the detriment of tear factor. Tear is more sensitive to refining than to pressure but the effect of repulping decreases tear while at higher pressure repulping tear is increased. Overall, the tear factor response to these variables is the mirror image of those for burst.

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