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SOME FUNDAMENTALS OF PAPER AND BOARD ENGINEERING

Professor Douglas Wahren The Paper Professor AB Moränvägen 6 S-791 74 Falun, Sweden now retired, until recently: Senior Vice President Stora Corporate Research AB S-791 80 Falun, Sweden

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INTRODUCTION

In conventional product engineering the product functionality is to be optimized while costs are minimized. Various materials can be selected on the basis of well defined mechanical and other properties. The same can be said about the engineering of transport packaging and some other products in which paper or board may be selected as a component.

Knowledge of the requirements on paper and board components for various end uses is crucial to commercial success of the producer of these materials. Producers also need to minimize the costs for meeting the demands precisely. The paper and board engineer is faced with the task of engineering a sheet or web <u>material</u> which the end user – or end product designer – will select based on performance, i.e. properties, and price.

The objective of the paper and board engineering system presented here is to enable the developer to do most of this on the computer. Once the sheet design and the composition of the furnish(es) seem to fulfill the user's requirements any experimental work may focus on these designs. This system has been used in STORA for a number of years and provided significant reductions of time to market and cost of development work. The development of the engineering system continues.

Basic Concept

This paper deals with the conceptual underpinnings of a system to calculate mechanical and optical **properties** of <u>sheets</u> consisting of <u>layers</u> made from <u>furnishes</u> which are <u>mixtures</u> of pulps, fillers and dyes. Formulas used for processing by refining, pressing, and calendering are included. The procedure used for pressing and calendering multi-layer sheets is indicated.

The type of phenomena dealt with is illustrated in the following diagram.



Figure 1. Tensile Stiffness Index of an uncalendered Printing and Writing paper as a function of the filler content. The base paper is a 50/50 mix of NBSK and NBHK, and the filler is China Clay, grade C. The thick full line represents the assumption that the volume concentration, **C**, of solids in the sheet is unchanged. The thick, dotted line is calculated on the assumption that the apparent density, **D**, of the sheet is constant, i.e. its thickness is the same after adding the filler as it was before.

A printing and writing paper base was filled to various levels with Grade C clay. The Tensile Stiffness Index (**TSI**) and other properties were measured. Plotted in *Figure 1* are the measured **TSI** values for 0%, 15%, and 25% filler content.

Three lines are drawn in the diagram. The thin, full line represents the decrease of **TSI** that would be expected based only on the reduction of the amount of fiber due its replacement with filler, assuming that the filler is inert. Obviously, this simple scheme is not enough to explain the actual reduction of **TSI**.

The two thicker lines (curves actually) take into account not only the replacement of fiber by filler but also that the <u>fiber network is diluted</u>, i.e. that the mass of fibers per unit volume of paper is reduced. In doing so one has to assume, or otherwise establish, what the volume of the paper is after filling.

The thick, dotted line is calculated on the assumption that the apparent density of the sheet is unchanged, i.e. its thickness and basis weight are the same after adding the filler as it was before. This implies that the bulk of the fibrous component has increased, i.e. that the apparent density of the fibrous component has decreased. The thick, solid line represents the assumption that the volume concentration, C_v , of solids in the sheet is unchanged. This means less of a loss of <u>fiber</u> network density (bonding) than the first assumption. Reality is usually in between.

In both cases the reduction of **TSI** has been calculated as a function of the apparent density of the fiber network after "dilution" with inert filler. The basis for the calculation is a series of measurements of **TSI** of unfilled base paper subjected to wet pressing to various levels.

The diagram is only an illustration and as such does not prove anything. As it turns out, however, this general line of reasoning holds up well enough and can be expanded far enough to provide guidelines for storage and treatment of data to make them useful for paper and board engineering purposes.

Scope

The paper and board engineer has at his/her disposal a large or limited number of pulps, fillers and dyes and a multitude of processing steps such as refining, mixing, forming one or several layers from various or variously treated and mixed furnishes, pressing, drying, coating, calendering, and laminating. Add also the broke generated in the process, calculation of its properties, and various ways of including it in the sheet and this is the basic list of functions addressed in this paper but only insofar as their influence on product properties go – and the associated costs.

Each layer of the sheet may include one or several pulps, fillers, shading colors etc. in any proportion. The components - and the composite - may be mixed, refined, pressed, calendered, shaded etc. The range of validity may be made as wide as required.

Coatings and laminating materials are just added with their measured properties and are not processed from scratch.

The properties considered here are all optical properties (including formation/mottle) and all elastic properties and their derivatives such as tensile and bending stiffness. Strength properties are *not* included for the time being nor are rheological or time dependent effects. Costs are treated too but only to provide the designer (not the accounting department) with a suitable foundation, particularly for considering the large influence of broke on costs and properties.

Among functions that are not addressed are any and all chemical properties, the use of process chemicals, profiles, slitting, winding, sheeting or any process details. The implicit assumptions are that equipment and processes are reasonably close to the state of the art or else that the user adjusts the input or output data to fit the particular situation.

The objective is to enable the developer to do much of the product development work on the computer, i.e. to put to good use measured data, our understanding of the fundamentals, and good engineering practices. The criteria are usefulness and practicality.

On the mechanical side the teachings of elementary structural mechanics are taken for granted, for instance methods to calculate the bending stiffness of a composite beam. On the optical side the Kubelka-Munk formulas are adopted straight from the textbooks. Neither type of basic formula will be reviewed here.

Testing

In order for such an approach to be valid, however, it is absolutely essential to adopt measuring methods that provide relevant data. Hence, caliper is measured according to the STFI method (1, 2), and an Elrepho 2000 reflectometer (3) is used for the optical measurements. The Tensile Stiffness Index (TSI) is determined according to (4). These are as close approximations to the theoretically correct methods of measurement as have been possible to find – and they work.

Each material (pulp, filler, dye, etc.) to be used in the calculations has to be characterized with respect to its basic mechanical and optical properties – including the influence of refining, pressing, and calendering over sufficiently wide ranges. The measured data is used to describe multidimensional property surfaces along which the required properties can be read exactly or interpolated.

It was found through extensive experimentation that the elastic and optical properties of most papermaking materials are "well behaved" in the sense that all changes are gradual and continuous so that the data can be described by simple functions; power functions of apparent density were selected. This good behavior does not extend to all strength properties, however.

In practice, the measured data is collected in a database from which the user selects whatever materials are desired. The user elects how to combine various materials, how to structure the sheet, and how to process it.

Completely transparent to the user, a computer program might then use the "property surfaces" for interpolation to the right processing conditions and uses the mixing rules described below. In a second or less all properties and costs of the product are calculated.

More or less sophisticated optimizing schemes might be employed to assist the user in finding an optimum or an optimum range to be validated by limited experimental work. Thanks to the virtually instantaneous response, however, most users find it convenient enough to "feel their way through the maze" – the computer providing instantaneous feedback as they try various ideas.

Turning the problem around it is also possible to compare the performance of specific pulps or fillers, etc. in a particular product to put an economic value on these materials.

Structure of this Report

Engineering paper and board in the computer requires good, quantitative data and mathematical descriptions of how the data may be combined and used. This is a kind of "chicken and egg" problem: the model requires measured data and the measured data must be usable in the model. Standard pulp and paper testing methods were not developed with computer modeling in mind. Although many standard methods are usable evaluation of processing and testing methods has been an integral part of the project. Feedback from colleagues in development departments in the mills was (not always complimentary but) invaluable in this context.

Because discussions of the crucial processing and testing methods do not require knowledge of the mathematical models I have elected to discuss the processing and testing methods before going into the mathematical descriptions. The real development in the two areas occurred in parallel and was highly interactive.

The mathematical descriptions are stated as they would be used in modeling a sheet. In order to utilize fully all the information in the experimental data the loop must be closed, i.e. the experimental data must be evaluated in the same modeling terms. Model parameters are forced to fit experimental data. If the fit is good then the data is accepted and that part of the model is automatically verified. If the fit is not good then the data is rejected or additional, more closely spaced, experimental data obtained until the fit is good enough. This is discussed briefly.

Other parts of the model, such as mixing rules, need conventional experimental verification. A few illustrations of such verifications are provided.

MATERIALS PROCESSING AND TESTING

Pulp Processing

The generally good behavior of pulp properties as functions of density can be utilized to limit routine experimental work. When no surprises are expected satisfactory information is obtained by evaluating a pulp at three refining levels times three wet pressing levels. Calendering requires, at a minimum, three levels of calendering. This normally done on the medium refined and medium pressed sheet. Thus, the minimum level of sheet making comprises 9 different sheets plus 3 - 6 extra for the calendering operations. Testing is then limited to 12 differently treated sheets with whatever replication of samples is required by the particular tests.

The particular processing and testing methods referred to in this report are the ones which we have found to provide the most useful data, i.e. they can be used with reasonably high confidence that state-of-the-art industrial products would have properties quite close to the ones predicted.

Other processing and testing methods can be used as long as they are internally consistent but their value would be limited to <u>relative</u> comparisons, and even so the effects of industrial refining might be surprising. In any case, the model becomes invalid if data derived from different standards are mixed. A specific problem is that, for homogenous materials with a rectangular cross section, the caliper must satisfy the conventional relation between tensile and bending stiffness:

$$\mathbf{BSI} = \mathbf{TSI} / 12\mathbf{d}^2 \text{ or } \mathbf{t} = [12\mathbf{BS} / (\mathbf{W} \cdot \mathbf{TSI})]^{1/2}$$
(1)

where **BSI** is the bending stiffness index, **TSI** the tensile stiffness index, **d** is the apparent density, **t** is the caliper, and **W** is the basis weight.

On the practical side it might be noted that relevant comparative modeling can be done using any processing standard. In the early stages, for instance, we produced useful comparisons using industrial refining and standard handsheet making and processing. The absolute levels of some properties were off but the comparisons were good.

Refining

Refining is the most powerful method we have for enhancing pulp properties. My knowledge of the fundamentals of refining and refiner-fiber actions and interactions is too limited to be of any real quantitative, predictive value. Hence, the refining operation has to be carefully selected to represent the best available industrial technology (BAT) rather than any laboratory method which is capable of developing the ultimate strength (or other property) potential of the pulp. The difference in properties between a PFI and a BAT refined pulp is often of the order of 25% or more. Instances have been found, however, when industrial refiners have processed pulps to the same stiffness levels as were found using the PFI mill. Many industrial refiners perform less well than BAT refiners. This can only be known locally and has to be adjusted accordingly.

We have found that a well maintained and adjusted Jylhävaara JC-00 or an Escher-Wyss laboratory refiner can be used to represent a BAT refiner with sufficient accuracy and repeatability. It must be noted, however, that the particular refining tackle, the edge load, consistency, and other operating conditions have to be carefully controlled, and not necessarily to the same values for different refiners. We have found that one edge load / tackle combination can be used for treatment of softwood kraft pulps and another for softwood sulfite and hardwood kraft pulps. Other raw materials and other processes may necessitate other conditions to simulate the results of industrial operations.

Mechanical pulps have been sampled at various stages in mills. No good, small scale BAT refiner for mechanical pulps has been identified.

Sheet Processing

Again, the objective is to produce sheets that have the same properties as sheets produced on industrial state-of-the-art equipment. The two most influential properties which are controllable in sheet processing are the density after forming, pressing, and drying and the shrinkage during drying. We have built a piece of equipment which can be adjusted to simulate reasonably well the pressing and drying processes. It comprises one drying cylinder (diameter 0.65 m) wrapped (about 200°) by a synthetic felt with controllable tension.

A press roll (diameter 0.23 m) with controllable line load is loaded against the felt where it enters the dryer. In routine operations one standard felt tension and three press loads are used. The loads are selected to cover a somewhat wider range of density of the final sheet than is expected to be encountered in practice. Three press loads have been found to be sufficient to cover all but the most extreme conditions. The drying time is standardized to one minute and the dryer temperature and felt tension to values which, in combination with a blotter (or a piece of cardboard for very smooth sheets), provide the "right" shrinkage and thorough drying. The sheet is conditioned and tested at 50% RH and 23°C.

The sheet forming method employed has been found to be less influential on the properties than the pressing and drying conditions. It has been found to be very rational and practical to use a Formette Dynamique (5) because then only 12 or 15 sheets need to be made for a complete test series. It also serves to indicate the orientation potential of the pulp.

Processing of Fillers

Fillers must be tested "in context", i.e. in a sheet, in order to provide relevant information on how well they function in a sheet. We have found, fortunately, that if the proper procedures for evaluation (described below) are employed the composition of the "base paper" exerts very little influence on the results. Since many fillers have very low light absorption (**k**) values it is necessary to use pulps with very low **k** values to make the filler **k** values significant. We use as a standard a 50/50 mixture of Stora 32 (NBSK) and Stora 61 (NBHK) pulps refined to 25°SR and 22°SR respectively.

Sheets are formed in the Formette Dynamique and processed as described above but using 0.1% Percol 140 as a retention aid at all filler levels. The water used in forming is de-ionized and the conductivity adjusted with salts to a constant value.

A minimum of four filler levels are used, approximately: 0, 7, 15, and 25% but sometimes five or six levels are used and the range may be extended. The amount of filler actually retained in the sheet is measured as part of the testing routine. Hence, the computer simulation of a product may indicate that 10% filler should be used but it is up to the user / papermaker to make certain that this amount is actually retained in the sheet or layer.

One particular problem is that the absorption coefficients of some fillers are very low even compared to highly bleached pulps. Hence, reliable data may be difficult to obtain. An effective method to get around this obstacle has been developed. It builds on the Kubelka-Munk concept that light absorption power, i.e. light absorption coefficients times the amount (basis weight, concentration) of the material, are additive. Mixing in various fractions (FC) of filler in a base pulp then:

$$\mathbf{k}_{sheet} = FC \bullet \mathbf{k}_{filler} + (1 - FC) \bullet \mathbf{k}_{pulp}$$
(2)
or
$$\mathbf{k}_{sheet} = \mathbf{k}_{pulp} + FC \bullet (\mathbf{k}_{filler} - \mathbf{k}_{pulp})$$
(3)

so, if the absorption value of the filled sheet is plotted against the filler content, FC, then the slope of the line will be ($\mathbf{k}_{\text{filler}}$ - \mathbf{k}_{pulp}). The base pulp and the sheet basis weight can be chosen so that very reliable values of $\mathbf{k}_{\text{sheet}}$ can be evaluated. One example of such a plot is shown here.



Figure 2. The X, Y, and Z light absorption coefficients of **sheets** made from bleached pulp with varying contents of Grade C China Clay filler is plotted against the filler content.

Processing of Dyes

The few pigment-based dyes we have worked with could be treated as fillers.

Soluble dyes can present problems dues to varying requirements on the papermaking chemistry, and in a few cases it has been necessary to adjust the conditions to simulate those obtaining in the mill. One problem is to determine the exact amount of dye actually retained. A successful but rather labor intensive method solved this problem by incorporating the dye in a white coating formulation which was dried slowly and completely. We have now developed reliable methods that use ordinary spectrophotometric analyses of dyes in solutions. The key is controlling the chemistry of the solutions.

Processing of Coatings

Appropriate processing and testing of coatings is difficult and worth its own treatment. Suffice here to say that we have tried a number of methods and settled, for the time being, on coating a semitransparent drafting base with several different basis weights of coating. This makes it possible to evaluate the intrinsic optical properties of the coating. The same samples plus a few others made on different substrates are used for evaluation of the mechanical properties of the coating. These techniques need further development to provide data which can be used with a high degree of confidence. The "interaction layer", or rather the migration of binder within the coating layer and into the base confuses any generalized interpretation of data. In any specific case, however, it is possible to produce a simulation that accurately represents the experimental data and can be used in the particular context.

MODELING OF BASIC PROPERTIES

Density and Volume Concentration

The most basic properties of a layer are its basis weight, $W [kg/m^2]$, apparent density, $d [kg/m^3]$, and volume concentration, C_v [fraction]. The apparent density is d = W / t,

where t is the caliper (thickness) of the layer. The volume concentration of solids, C_v , is:

$$\mathbf{C}_{v} = \left[\mathbf{W}_{pulp} / \mathbf{d}_{pulp} + \mathbf{W}_{filler} / \mathbf{d}_{filler} + \mathbf{W}_{dye} / \mathbf{d}_{dye} \right] / t$$
(4)

where W_{pulp} is the (partial) basis weight of pulp in a layer, t is the layer thickness, $d_{pulp} = 1,500$ kg/m³, and d_{filler} and d_{dye} are the solid density of the filler and dye solid materials respectively. The STFI caliper, t [m], is used to calculate the apparent density.

Elastic Properties

The basic elastic parameter of a single layer is the elastic modulus, E [N/m²], from which is computed the Tensile Stiffness Index,

$$\mathbf{TSI} = \mathbf{E} / \mathbf{d} \quad [\text{Nm/kg}] \tag{5}$$

Empirical data are described by the relations which have a base in theory but which are simplified for ease of computational use.

$$\mathbf{E} = \mathbf{E}_{\mathbf{0}} \bullet (\mathbf{d} / \mathbf{d}_{\mathbf{0}})^{\mathbf{n}}$$
(6)

Here and below the subscript "o" (as in E_o and d_o) refers to **measured** variables. The exponents, e.g. **n**, are directly evaluated from measured data. Other variables are computed or exemplify computational procedures.

Hence, \mathbf{n} , \mathbf{d}_0 , and \mathbf{E}_0 are measured reference parameters for the sample. They usually describe the connections between \mathbf{E} and \mathbf{d} quite well for a particular pulp undergoing treatment. The exponent, \mathbf{n} , is different for refining, pressing, and calendering and is, in general, not a constant but a local

$$\mathbf{E}_{\text{treated},1} = \mathbf{E}_{o.DB} \bullet (\mathbf{d}_{\text{treated},1} / \mathbf{d}_{o.DB}) \text{Mechanical.Treatment.Exponent}$$
(7)

The term Treatment is used to represent refining, pressing, or calendering. There is sometimes confusion with regard to these exponents. It is quite common to use the tensile stiffness index (**TSI**) instead of the modulus of elasticity (**E**). Both conventions are equally valid. In order to keep track of the numerical values of the exponents, however, it is necessary to stick to <u>one</u> convention.

Since

$$\mathbf{TSI} = \mathbf{E} / \mathbf{d} = \mathbf{E}_0 / \mathbf{d}_0 \bullet (\mathbf{d} / \mathbf{d}_0)^{\mathbf{n} - 1}$$
(8)

there is a difference of one unit between the two conventions.

If the Formette Dynamique is used, or some other former which imparts an orientation to the sheet, then the properties in the Machine Direction (MD) and in the Cross Machine Direction (CD) are noted separately: $E_{e,MD,BB}$ and $E_{e,CD,BB}$. When using directional properties use is made of the relation (6):

$$\mathbf{E}_{\text{mean}} = (\mathbf{E}_{\text{MD}} \bullet \mathbf{E}_{\text{CD}})^{1/2} \tag{9}$$

Optical properties

The Kubelka-Munk notions of light scattering and light absorption are used but are based on basis weight rather than thickness. This was suggested by Johannes van den Akker and Åke Stenius and has been accepted by the paper industry and their customers (3). The standard reference for formulas and tabulated values etc. is (7).

The light absorption coefficient, $\mathbf{k} [m^2/kg]$, is assumed not to be influenced by refining, pressing, or calendering. By and large this assumption has been verified by our data but very white (low \mathbf{k} value) furnishes and sheets are easily contaminated, for instance by corrosion products in pilot refining systems or by "oil smoke" in the vicinity of hot calenders.

parameter. Hence, we use:

Densification does influence the light scattering coefficient, s $[m^2/kg]$ but, in extreme cases, the apparent density was found to be a less than suitable parameter for normalizing the data. Light is scattered at interfaces between materials with different indices of refraction. Light is not scattered if the distance between two surfaces is less than some fraction of the wavelength of the light. Hence, the pore size distribution must be considered. Just as in the case of the modulus of elasticity, however, we do not need some generally valid constant or model, just a local parameter describing the relevant data. Given a certain material (a layer of pulp or of a mix) having a certain pore size distribution the simplest measure relating to the change of pore sizes on densification is the solid fraction which is the same as the volume concentration, C_v of solids. The light scattering surface area would be some function of the pore fraction, i.e. 1 - solid fraction. This function will do, so the following function is adopted:

$$\mathbf{s_{treated}} = \mathbf{s_0} \bullet [(1 - \mathbf{C_{v,treated}}) / (1 - \mathbf{C_{v,0}})]^{\text{Optical.Treatment.Exponent}}$$
(10)

Here $C_{v,o}$ and s_o are reference parameters for the sample. The term Treatment is used to represent refining, pressing, or calendering. The light scattering and absorption coefficients have been measured and stored at three ranges of wavelengths corresponding to the X, Y, and Z filters.

This necessitates standardization of the light source, however, and limits the future general applicability of the data. Today, the s and k values are evaluated at 16 wavelengths. The user may then select the light source and display the color most relevant to the application at hand. Measuring and storing 16 or more wavelengths also provides the option to display and put numbers on metamerism.

Evaluation, Verification, Validity: 1. Test Data Representation.

Can one afternoon or a couple of days of modeling exercises replace hundreds and hundreds of hours of laboratory work and months of waiting for the results? ("If it sounds too good to be true then it probably is....") Obviously, the question of validity is foremost in the user's mind. Here we look at pulp data and their representation as described above. Other issues are dealt with in other sections.

It is assumed here that the refining, sheet making, pressing, and drying processes have been well selected and verified against good industrial data. It is also assumed that the processes are operated according to well prepared instructions, and that the same holds true for the testing methods.

The data is represented locally and forced to fit the model. Provided the fit is good enough this procedure is just one way of representing the actual data. Since, for "well behaved" materials (and high quality measurements) the measure of fit depends only on the spacing of the experimental points, this part is under the control of the investigator. If the range is too wide or the spacing too large to accommodate unusually steep changes then new experimental data can be added (or the user advised of the lack of accuracy).

As a matter of fact, since the investigator is treating all the data to adapt them to the functions just described, all the tools are available to detect any inconsistencies in the data. It happens, therefore, that spurious values are detected, traced back to the source, and corrected. The accuracy of the data representation in itself can be as high as required. In my experience, individual data points are rarely off more than about 1 percent from the original, tabulated values. Thus the relevance is not limited by the way the data is represented and stored but by the relevance of the processing methods employed – the refining method in particular.

No physical significance should be attached to individual coefficients and exponents – particularly not when the range of data is narrow or the number of data points is economically low. In certain cases, such as when characterizing a pulp or mixture that is going to be used for characterizing filler properties, the range should be wide and the experimental points closely spaced so that the "Treatment.Exponents" are accurate.

PROPERTIES OF MIXTURES

Most furnishes consist of two or several components so mixing rules have been developed to provide reasonably accurate and easily workable approximations. One fundamentally important concept used here is to keep track of each individual component of each furnish and to calculate the composite properties from scratch each time any component or processing step has been changed. Hence, there will be no accumulation of computational or approximation errors.

Equally important, however, is that each type of component (fiber, filler, dye) is represented and treated separately throughout. Hence, it is possible to keep the treatments of various components separate and apply the mixing and treatment rules and computations in the correct order.

The basic order is: Refining, Mixing, (Refining), Pressing, Calendering

At the user's discretion refining may be carried out separately or on a mixture of pulps or both. In all cases, however, the computations are made from scratch and the refining action is exerted only on the pulp component(s). Then the fillers and dyes are mixed in.

Similarly in the treatment of multi-layer sheets, pressing and calendering may be carried out on individual layers, for which one may have good empirical data on the effects, or on all layers simultaneously as would occur in practice. The procedures may also be combined so that the empirical knowledge is used where it is available and the model takes care of the rest.

So, from a modeling point of view each layer may have up to three basis weight specifications: one for pulps, one for fillers, and one for dyes.

Simple Additive Properties

Some properties are simply additive. Basis weight, light absorption coefficients, and raw materials costs belong in this class. For basis weights for instance:

$$\mathbf{W}_{\text{tot}} = \mathbf{W}_{\text{pulp}} + \mathbf{W}_{\text{filler}} + \mathbf{W}_{\text{dye}} \tag{11}$$

and light absorption coefficients:

$$\mathbf{k}_{\text{tot}} = \left[\mathbf{W}_{\text{pulp},1} \bullet \mathbf{k}_{\text{pulp},1} + \mathbf{W}_{\text{pulp},2} \bullet \mathbf{k}_{\text{pulp},2} + \mathbf{W}_{\text{filler},1} \bullet \mathbf{k}_{\text{filler},1} + \mathbf{W}_{\text{dye},1} \bullet \mathbf{k}_{\text{dye},1} \right] / \mathbf{W}_{\text{tot}}$$
(12)

Density and Volume Concentration

The basis weight of layer i is $W_{tot,i}$, which is the sum of the basis weight of the various pulps, fillers and dyes mixed into the furnish of the layer. One initial task is to calculate the density of each layer, i, made from this furnish. **The basic assumption** made here is that the **volumes** of the pulp fractions **are additive** (8). This translates into:

$$\mathbf{d}_{\text{Mix},i} = \mathbf{W}_{\text{tot},1} / \left[\mathbf{W}_{i,1} / \mathbf{d}_{o,\text{DB},1} + \mathbf{W}_{i,2} / \mathbf{d}_{o,\text{DB},2} + \dots + \mathbf{W}_{i,n} / \mathbf{d}_{o,\text{DB},n} \right]$$
(13)

Here $\mathbf{d}_{o.DB.n}$ is the density given in the database for pulp **n** of layer **i** or it may be a density achieved by "refining in the computer" of that pulp. Knowing the density and composition of the mixture the volume concentration of the mixture can be worked out. Hence, there is sufficient data to compute both the mechanical and optical properties of each pulp fraction.

It should be emphasized that the **density of the mixture is fundamental** to the model and all calculations. The next step is to calculate the properties at this density and the corresponding volume concentration, and then go on to model further property development by pressing and calendering.

The volume concentration, $C_{v,Mix,i}$, of the layer i is:

$$\mathbf{C}_{\mathbf{v}.\mathbf{mix.i}} = \left[\sum_{x} \mathbf{W}_{\mathbf{pulp}} / \mathbf{d}_{\mathbf{pulp}} + \sum_{x} \mathbf{W}_{\mathbf{filler}} / \mathbf{d}_{\mathbf{filler}} + \sum_{x} \mathbf{W}_{\mathbf{dye}} / \mathbf{d}_{\mathbf{dye}}\right] / \mathbf{t}_{\mathbf{i}}$$
(14)

where $W_{pulp,x}$ is the (partial, fraction x, summation over x) basis weight of pulp in a layer, $d_{pulp} = 1,500 \text{ kg/m}^3$, and d_{filler} and d_{dye} are the solid density of the filler and dye respectively.

Elastic and Optical Properties

The contribution of Pulp \mathbf{x} to the modulus of elasticity, \mathbf{E} , and the light scattering coefficient, \mathbf{s} , is calculated as follows.

$$E_{i,Mix,x} = E_{i,Refined,x} \bullet (d_{i,Mix} / d_{i,Refined,x})^{Mechanical.Pressing.Exponent.x}$$
(15)

$$s_{i,Mix,x} = s_{i,Refined,x} \bullet [(1 - C_{v,i,Mix}) / (1 - C_{v,i,Refined,x})]^{Optical.Pressing.Exponent.x}$$
(16)

The contributions of each pulp to the properties of the mixture are linearly weighted and summed.

The sensitivity exponents (Mechanical.Pressing.Exponent, etc.) of the mixture are also linearly weighted and summed. Within the normal realms of papermaking the exact form of the relation used for the exponent weighting does not influence the results much.

Fillers

There has been plenty of speculation of how fillers interfere with bonding but no definite and generally applicable theory exists. The present approach takes as a starting point the assumption that fillers have mass but are completely inert. In that case two effects would come into play:

- a) Reduction of Tensile Stiffness Index (TSI) and TI in proportion to the degree of substitution, and
- b) Reduction of **TSI** and **TI** due to the lower concentration (apparent density) of the fibrous part of the sheet. This latter factor has by and large been ignored in the past.

In this simple mechanistic line of reasoning the computation of effect a) is trivial.

Computation of effect b) requires knowledge how much the fiber network density changes when filler is added. There are two <u>simple</u> (remember Occam!) possibilities: 1) No change of density, and, 2) No change of volume concentration. Experiments show that, at constant refining and pressing conditions, the actual results usually fall somewhere in-between these two extremes. At low filler contents the two are indistinguishable. At high filler contents approximation 1) tends to underestimate and approximation 2) to overestimate the density.

Question b) also requires knowledge of how the fiber network properties change with density when the fibers keep their properties. The obvious way to find out is to change the sheet density by pressing. In fiber network studies the total effects on stiffness and strength are often well approximated by a power function of the apparent density, and that seems to apply quite well to wet pressing data – provided the drying conditions are well controlled and constant. This line of attack results in the following rules.

Rule no. 1: When a filler is added to a furnish the apparent density of the sheet or layer does not change.

As experimental data has accumulated it seems that assuming constant volume concentration instead of density may be a slightly better indicator at high levels of pressing and calendering. The actual value used is decided by the investigator.

Rule no. 2: With exception of Rule no. 1 the mixing rules used for pulps apply.

So, when filler is added to a furnish two primary things happen:

1. Pulp fibers which normally provide strength and stiffness are replaced by a more or less inert filler. Hence, strength and stiffness drop.

2. The pulp fiber network is diluted because, according to **Rule no. 1**, the layer density remains the same but "strength-effective" pulp fibers are replaced by filler particles. Hence, the effective density of the fiber network is lowered.

These rules imply that the fillers do not form networks or other structures with measurable strength, elasticity, or density. The fillers place themselves more or less in the voids between the fibers. The **basic assumption** made here is that the **fillers are inert**.

This has been shown to be a very good approximation for papermaking clays, and it is a reasonable first approximation for other fillers. Corrections can then be made. These rules and primary effects are sufficient to explain most of the effects of filling a sheet with ordinary papermaking fillers:

- The strength and stiffness drop because there are fewer fibers per kilogram of paper and because the fiber network has a lower effective density.
- The light scattering power increases thanks to the higher scattering coefficient of the filler and because the fiber network has a lower density and volume concentration which increases the unbonded area and, hence, the light scattering coefficient of the fibers.

In many cases there are also secondary effects. With respect to mechanical properties ordinary papermaking clays follow the above rules quite closely, i.e. as if they were totally inert or contributing very slightly to the strength and stiffness. Some other pigments, notably the PCCs tested so far, exhibit a negative influence on the mechanical properties over and above what is calculated according to the above rules. The reason for this is not known it may be an influence of the dispersants used or it may be a case of the filler actually interfering with fiber bonding. This influence is noted as a positive or negative contribution to the modulus of elasticity which is included in the model.

The Complete Layer

The elastic and optical properties for a layer can now be computed:

$$\mathbf{E}_{i.Mix} = [\mathbf{W}_{i.1} \bullet \mathbf{E}_{i.Mix,1} + \mathbf{W}_{i.2} \bullet \mathbf{E}_{i.Mix,2} + \dots + \mathbf{W}_{i.n} \bullet \mathbf{E}_{i.Mix,n}] / \mathbf{W}_{tot.i}$$
(17)

$$\mathbf{s}_{i.Mix} = \left[\mathbf{W}_{i.1} \bullet \mathbf{s}_{i.Mix,1} + \mathbf{W}_{i.2} \bullet \mathbf{s}_{i.Mix,2} + \dots + \mathbf{W}_{i.n} \bullet \mathbf{s}_{i.Mix,n} \right] / \mathbf{W}_{tot.i}$$
(18)

$$\mathbf{k}_{i.Mix} = \left[\mathbf{W}_{i.1} \bullet \mathbf{k}_{i.Mix,1} + \mathbf{W}_{i.2} \bullet \mathbf{k}_{i.Mix,2} + \dots + \mathbf{W}_{i.n} \bullet \mathbf{k}_{i.Mix,n} \right] / \mathbf{W}_{tot.i}$$
(19)

Since the light absorption coefficient does not change during processing equation (18) is in effect identical to eq. (12).

Evaluation, Verification, Validity: 2. Mixtures

Obviously, evaluation of characteristic data for pulps will consist of suitably spaced experimental grids dealing with refining, pressing, and calendering. The basic parameter controlled by these processes is the sheet density. The dependent parameters illustrated here are the Tensile Stiffness Index and the light scattering coefficients. The necessary light absorption coefficients are evaluated too but usually "reconciled" to a constant value for each pulp – provided of course that the experimental conditions justify such a procedure.

In the neighborhood of each experimental point the "Mechanical.Treatment.Exponents" and "Optical.Treatment.Exponents" relating mechanical and optical properties to the density are evaluated. In conjunction with the absolute values at each experimental point a complete description is obtained.

Fillers and dyes are evaluated when mixed into suitable "base pulps" or pulp mixes with known properties. The contributions by the fillers and dyes to the properties of the mixtures, above and beyond what is given by the basic "mixing rules" is noted as their respective contributions to properties. Unpublished experimental investigations by Mikael Alexandersson have shown that the specific nature and properties of the "base pulp" has only minor influence on the results evaluated – provided of course that the pulp used has low enough **k** values compared to the material being investigated and is stiff or strong enough to permit exposure of influences on the mechanical properties.

A typical example, data taken from such an investigation, is shown in Figure 1.

It is also possible, although more involved and requiring more data, to evaluate individual property contributions by various components in mixtures from experimental data on mixtures having various known compositions. This is inconvenient but may be necessary to do on occasions where pure materials are not available. This may be the case for instance with recycled pulps.

For a minimum demonstration of validity it now remains to show that the "mixing rules" apply to pulps.



Figure 3. The Tensile Stiffness Index of mixes of a low freeness SC magazine groundwood pulp and a Northern Softwood Bleached Kraft pulp (NIST reference NSBK).

For a simple demonstration two very different pulps were selected. One was a low freeness (39 mL) groundwood used in the production of SC magazine grades. The other was the National Institute of Standards NBSK reference pulp. This pulp was only lightly refined (to 25°SR) in the PFI mill. Other refining levels were tried too as were uncalendered and more heavily calendered sheets of varied compositions.

The results shown in *Figure 3* are typical – fortunately, it doesn't get much more "interesting" as far as optical and elastic properties are concerned. Data is usually quite well behaved, and if not then a closer scrutiny may be in order. Exceptions to this good behavior are effects of the <u>first</u> hard calender nip on papers with a high (90+%) content of mechanical pulp. Property changes between the first and the following calender nips are usually quite well behaved, i.e. they are valid <u>locally</u> but not in the transition from the uncalendered to the calendered state. Once some desired state has been reached by "processing in the computer" it is always advisable to check this data against the closest experimental data points available. Strength properties still surprise me on occasion, but that is another story.

Figure 4, is the companion optics illustration to Figure 3. The correlation is not very good but this is a fairly extreme case and completely unretouched. It was selected because it refers to the data set underlying Figure 3. Many data representations of mixes that have been investigated are better but even this one is good enough for establishing whether or not any particular mix might be of interest for a more detailed study. Remember that the intention is not to "do science" but to assist engineers in weeding out quickly 90% or more of unnecessary laboratory work.



Figure 4. The light scattering coefficient (Y filter) of mixes of a low freeness magazine groundwood pulp and a Northern Softwood Bleached Kraft pulp (NIST reference NSBK).

DERIVED PROPERTIES

Provided the experimental data are of high enough quality, and that they are well represented by characteristic, local parameters, any number of composite properties of various products can be calculated. In this context, the derived properties of most interest are usually tensile and bending stiffness, reflectance and transmittance factors, opacity, $L^*a^*b^*$, Whiteness, etc. of layers and sheets. Included here are also the optical effects of formation.

Bending of Multi-layer Sheets

Since bending stiffness is a very important and basic property of many multi-layer designs including most carton board products the cross section and tensile stiffness of each layer may be, and usually is, different. Using the knowledge of the properties of the individual layers the bending stiffness of the composite sheet can be calculated.

Each layer contributes to the bending stiffness in two ways, namely, by the bending stiffness of the layer itself and by the fact that most layers are situated a distance away from the neutral line, i. e. the line (or plane) along which bending occurs - and where the tensile stress due to the bending deformation is zero. This is the elegant idea behind the I-beam and stiff multi-ply board.

The bending stiffness of a single layer is $\mathbf{E} \cdot \mathbf{I}$ where \mathbf{E} is the modulus of elasticity and \mathbf{I} is the moment of inertia of the cross section. For a beam having a rectangular cross section:

$$I = B t^3 / 12$$
 (20)

where **B** is the width of the beam and t is its thickness or height. In paper mechanics the convention is to use the bending stiffness per unit width:

$$\mathbf{S} = \mathbf{E} \mathbf{I} / \mathbf{B} = \mathbf{E} \mathbf{t}^3 / 12 \tag{21}$$

In principle, then, one must calculate the bending stiffness of the individual plies, find the neutral plane, and then add the contributions due to the offset of various plies from neutral. This can be quite tedious. One rather elegant and efficient computing scheme for the total bending stiffness is found in textbooks on structural mechanics:

1. Assume that bending takes place in a vertical plane and the paper or board is horizontal.

- 2. Change the width of each layer in inverse proportion to its modulus so that the product of the layer width and its modulus are the same for all layers. This reduces the problem from one where we deal with varying material properties to one where the modulus is constant but the geometry is irregular.
- 3. For a beam having uniform modulus the neutral plane is located at its center of gravity irrespective of the actual shape of the cross section. So, the next step is to calculate the center of gravity of the cross section obtained by the reductions mentioned in the previous paragraph. This is straight-forward for cross sections consisting of rectangles.
- 4. The total bending stiffness is now calculated as the sum of the individual bending stiffness of all the plies plus their contributions due to their offsets from the (now known) position of the neutral plane.

In the case of oriented sheets the calculations have to be performed separately in the machine and cross machine directions.

Reflectance, Brightness, Opacity, Transmittance, Tristimulus, L*a*b*, Whiteness

The reflectance factors \mathbf{R}_{o} , \mathbf{R}_{∞} , and the transmittance, \mathbf{T}_{o} for each single layer are computed by means of the Kubelka-Munk formulas. For each filter or wavelength, the values for \mathbf{k} and \mathbf{s} are noted for each layer, and \mathbf{R}_{o} , \mathbf{R}_{∞} , and \mathbf{T}_{o} , are computed. \mathbf{R}_{o} and \mathbf{T}_{o} for multi-layer sheets are then calculated using known formulas. Knowing \mathbf{R}_{o} and \mathbf{R}_{∞} for the whole sheet it is a straight forward task to calculate the values of Tristimulus, $\mathbf{L}^*\mathbf{a}^*\mathbf{b}^*$, Chroma, Hue, Whiteness, and Tint.

Modern PCs, monitors and programming languages make it a rather straight forward task to display the true colors on the screen, e.g. as a Top View, a Bottom View, and a Cross Section. As mentioned above, if **s** and **k** are known for at least 16 wavelengths then the possibility exists to let the user choose various light sources and actually view the different shades that may be generated – optical metamerism. Characteristic numbers can be generated too but in most cases seeing is what leads to real understanding.

Formation and Mottle

In multi-layer sheets, not least when considering coatings as layers in the sheet, one task of the designer is to minimize the influence of poor formation (usually of some layer that is known to be poor by necessity) on the overall uniformity of appearance of the product. In other instances the objective is to diagnose which layer contributes most to poor appearance of a product. To meet the first objective numerical measures are most useful, to meet the second visualization can be most effective.

In both cases one layer at a time is given a slight variation up and down in basis weight and the optical effects on $\mathbf{R}_{o,\text{Teep}}$, $\mathbf{R}_{o,\text{Bottom}}$, and \mathbf{T}_{o} are noted. Measures of the sensitivity are then computed:

Mottling sensitivity, top =	$(\Delta \mathbf{R}_{\mathrm{o.Top}}/\mathbf{R}_{\mathrm{o.Top}})/(\Delta \mathbf{W}_{\mathrm{i}}/\mathbf{W}_{\mathrm{i}})$	(22)
Mottling sensitivity, bottom =	$(\Delta \mathbf{R_{o.Bottom}} / \mathbf{R_{o.Bottom}}) / (\Delta \mathbf{W_i} / \mathbf{W_i})$	(23)
Mottling sensitivity, look-through =	$(\Delta \mathbf{T_o}/\mathbf{T_o})/(\Delta \mathbf{W_i}/\mathbf{W_i})$	(24)

Since the effects are rather small when developing a product which is good in this respect the measures are usually expressed as percent. The sign is always included since the reflectance values actually may go either way depending on the sheet design.

For diagnostic purposes more realistic (i.e. larger) variations are used. The effects are displayed on the screen and compared to the actual sample. This may be instructive; even a severely mottled appearance is not always caused by the outermost layer.

PRESSING AND CALENDERING OF MULTI-LAYER SHEETS

When modeling pressing and calendering of multi-ply sheets it is necessary to decide or to find out how the densification is distributed among the plies. Three methods are used:

- 1. Individual densification of each layer. This is the preferred method when machine or experimental data is available. Can be used on those layers where this is the case.
- 2. A method that builds on the assumption that all layers are subjected to the same compressive stress. This is the preferred method when detailed experimental information is not available. This method takes into account the large compressive strains involved in wet pressing and calendering. It is the default method used. The basic parameters are the ingoing volume concentrations of the layers.
- 3. Densification of all layers to the same volume concentration or pore fraction or solid fraction. This is easy to compute and to understand but has little to do with reality. It is sometimes useful as a starting point.

Notes of Caution and Background

Note that this method has been developed and selected primarily because among physically reasonable models it is the simplest.

Osakii, Fujii, and Kiichi (9) present a concept involving three-dimensional networks, their contact point density, and volumetric stress and strain concepts which, in essence, are quite close to the ones used here. They provide a couple of the very rare examples of experimental verification of the validity of this line of reasoning.

Dr. José J. A. Rodal (10) uses the logarithmic strain concept in calendering process applications and provides references back to Hencke and others.

Virtually all published theoretical treatments of calendering concern the process or the resulting properties – usually then for single layer sheets.

Conceptual Framework of the "Same-Stress-on-all-Layers" Approach.

Since layers in a sheet have negligible mass in comparison to the press or calender rolls, each layer is subjected to the same stress. In the case of high speed wet pressing of heavy sheets or layers dewatering forces are significant, however, and the fluid phase carries some of the stress. Such cases warrant special consideration and are not treated here.

When straining paper or board in the MD or CD fracture or buckling occurs after just a few percentage points of strain. In ZD compression, however, the strains can be very large. The conventional Hookean concept of stress as a function of strain is then less than useful: it always leads to "exponential-like" stress-strain relationships. A valid concept of <u>large</u> strains has to be incorporated. This is done here by using logarithmic strain (or General strain), a concept conventionally used with rubbery materials.

It is implicit in the following treatment that all strains are permanent. This is of course not a valid description of the processes. If the results of the processes are measured (the permanent densification) and used as input data for product characterization then this may be a sufficient approximation for predicting product properties. Experience with this model has shown that it serves rather well.

The compressive modulus of sheets or layers is usually not known. Pressing and calendering involve large strains in the thickness direction of the sheet. In such cases the volume concentration or solid fraction of each layer is the most reasonable and available measure of its resistance to compression.

So, the model uses the distribution of compression among the layers in a sheet by considering the large strains involved and assuming that the stress is the same on all layers and that the compressive modulus is related somehow to the solid fraction in each layer.

The General (or Logarithmic) Strain Concept.



Figure 5. Beaker with a fictive, porous, substance representing a fiber network at various compressed levels.

Imagine a beaker with a porous substance, call it a fiber network or a pulp as represented by *Figure 5*.

- If the network were fully compressed (to 1500 kg/m^3) it would occupy the space from the bottom up to height L_m .
- Compression starts at a lower consistency, i.e. when the pulp fills up to height L₀.
- The fiber network (pulp) is now compressed to height L.

For small strains, d:

$$d\varepsilon = dL / L_0 \tag{25}$$

Considering that the absolute maximum deformation is to L_m a better concept is:

$$d\varepsilon = dL / (L_0 - L_m)$$
⁽²⁶⁾

Integrating:

$$\varepsilon = \text{Log}\left[\left(L_0 / L_m - 1\right) / \left(L / L_m - 1\right)\right]$$
(27)

where Log is the natural logarithm. Considering that the volume concentration, C_v, is

$$C_v = L_m / L \tag{28}$$

one finds a useful measure of the strain:

$$\varepsilon = \operatorname{Log}\left[\left(1/C_{vo}-1\right)/\left(1/C_{v}-1\right)\right]$$
⁽²⁹⁾

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where C_{vo} is the initial volume concentration before compression. Thus, naturally, the strain is directly connected to the volume concentration of solids in the porous material. This is a definition of strain which, over the years, has proven itself useful in many contexts involving large strains.



Figure 6. General Strain as a function of Conventional Strain for values of $C_{vo} = 0, 0.25, 0.5, 0.75, and 0.9. The dotted lines indicate the locations of <math>1 - C_{vo}$ for each one of the curves. The "general strain" tends towards infinity at these levels of linear strain because this is where the volume concentration tends to 1.

Denoting conventional, linear strain by s it is easily shown that

$$\varepsilon = -\text{Log}\left[1 - s / (1 - C_{v0})\right]$$
(30)

This is the function plotted in the diagram above to show the numerical consequences of the concept.

It is seen from *Figure* δ that it is the general measure of **strain** which increases in exponential-like manner. The primary reason that most compressible materials exhibit exponential-like increase of compressive **stress** as a function of conventional ("linear") strain is that the **real strain** increases as shown in the diagram. This concept may be used as one base in research on pressing and calendering. The General Strain is always higher than the linear strain. They both start at zero and then $d\epsilon/ds > 1$.

The curves in Figure 6 may be compared, for instance, to the ones published by Schaffrath and Göttsching (11) for the compression of papers and plastic foils.

Compressive Modulus

Disregarding plastic deformations the compressive stress, P, now will be:

$$\mathbf{P} = \mathbf{E}_{\mathbf{z}} \cdot \mathbf{\varepsilon} \tag{31}$$

where \mathbf{E}_{z} is the modulus of elasticity (in compression) in the usual sense (Young's modulus). In calendering, however, plastic deformations are important – the structure is re-arranged – and the compressive modulus may increase with increasing compression. A common form (Ingmanson, Robertson in the 1950's) for describing this phenomenon at low pressures (compressive stresses) is:

$$C = C_0 + M \bullet P^N \tag{32}$$

where C stands for the mass concentration (kg/m³) and C is some low, initial value. At high pressures (where C_0 can be ignored) the relation may be re-written:

$$\mathbf{E}_{\mathbf{z}} = \mathbf{E}_{\mathbf{z}\mathbf{v}} \cdot \mathbf{C}_{\mathbf{v}}^{1/N} \tag{33}$$

where 1/N is in the range 2 to 3. This can be regarded as the background to the method employed here to include effects of plastic deformations.

Relative Densification of Layers in Pressing and Calendering

For the purpose of modeling the relative densification of various layers in an existing multi-layer web structure it is not necessary to know the exact values of N and E_{zo} . The following line of reasoning is then utilized.

First, the new, desired calendered density is established. Since the furnish composition and caliper of each layer is known the solid fraction, or the volume concentration, can be calculated. A theoretical caliper of the solids in each layer equals the product of the caliper of the layer and the solids fraction. The rest of the caliper is made up of voids. It is assumed that it is only the voids which are compacted by the calendering operation, i. e. the solid fraction, corresponding to L_m in Figure 5, can not be compacted.

As a measure of the modulus, E, use is made of the relation mentioned above:

$$\mathbf{E}_{z} = \mathbf{E}_{0} \cdot \mathbf{C}_{v}^{1/N} \tag{33}$$

but simplifying it into proportionality:

$$\mathbf{E}_{\mathbf{z}} \approx \mathbf{E}_{\mathbf{z}\mathbf{0}} \cdot \mathbf{C}_{\mathbf{v}}^{\mathbf{C}\mathbf{E}} \tag{34}$$

where CE is an exponent in the range 0 - 5. Theories of fiber networks put the value of CE between 2 and 3 with the lower value most probable for very slender fibers and the high end of the range most probable for stubby fiber debris or more or less spherical particles. The theoretical value of CE also depends on the degree of out-of-plane orientation of the fibers. A special case of it (CE=2) has been used with reasonably good results for at least five years. It is not backed up, however, by explicit experimental evidence. I hold today that CE = 2.5 is the best default value for the general case when no specific information is available. The differences are very small, however.

Combining now the compressive stress (eq. 31) with the expression for the general strain:

$$\mathbf{P} / \mathbf{E}_{z_0} = \mathbf{C}_{\mathbf{v}}^{\mathbf{CE}} \cdot \mathbf{Log}((1 / \mathbf{C}_{v_0} \cdot 1) / (1 / \mathbf{C}_{v_0} \cdot 1))$$
(35)

It is not necessary to know the value of \mathbf{E}_{so} or \mathbf{P} in order to use this formula to determine the distribution of densification among layers in a multi-layer sheet. The reason is that only the relative stress is used to obtain the distribution of densification. Only the right hand member of expression (35) is actually used in computations; when it is set equal for all layers the resulting volume concentration can be evaluated.

Here we can see that CE is a kind of sensitivity indicator: higher values of CE raise the relative resistance to compression of the densest layers. It can be demonstrated that the final outcome is only weakly dependent on the exact value of CE when CE > 2.

Turning the perspective around it is realized that if empirical data is available which relate the press or calender load to the volume concentration then it is possible to predict with some certainty the effect of a change of press or calender load on the volume concentration and, hence, on the density and all other properties.

BROKE AND ECONOMICS

The model of the Broke System is shown in *Figure 7*. Salable paper or board with one or more layers is produced at some rate which is set to unity. A fraction **B** of the quantity <u>produced</u> on the machine goes to broke and may be refined to enhance properties. The broke stream may be put into a single layer or may be split between two or more layers.



Figure 7. A sheet with one or more layers is produced at unity rate (kg/s, tons/h, etc. of salable paper). A fraction, **B**, <u>of the quantity run across the paper machine</u> goes to broke and may be given a strength or stiffness yield and /or may be refined to enhance properties.

The Broke Algorithm

The User decides on the fraction of broke, \mathbf{B} , and the fractions, \mathbf{p} , \mathbf{q} , of the broke stream to be put into each layer. Theoretically impossible values are weeded out in the process. Questions regarding technical or economical practicality are not addressed at this stage.

The composition of the broke stream is computed in two parts. First the composition of furnishes in layers which do <u>not</u> receive broke are determined.

For the layers that do receive broke the composition of the remaining parts of the furnishes, that pass straight through the process are determined. All these components are then mixed and the properties of the mixture are determined. These are the basic properties of the broke. Strength, stiffness, and light scattering "yield" factors are available that may be employed and calibrated according to local experience.

Depending on which layers receive the broke the net composition of the sheet and the "broke furnish" might change. The broke is now regarded as a furnish with known composition (including fillers, dyes, and remnants of coatings) and known properties.

The costs of the raw materials are included in these calculations in proportion to the **net** flows of each material into the sheet. Note that the net flow rates are adjusted so that they correspond to the total sheet basis weight (factor $[1 - B]^{-1}$).

The flows of broke into one or more of the layers have already been decided by the User. The remaining task then is to mix the appropriate amount of the "broke furnish" into each designated layer using the normal mixing rules described in other sections and to determine the properties of the mixture in each layer. The properties of the sheet can then be determined.

The Cost Algorithm

All properties are measured, calculated, and reported at standard climate conditions, i.e. 50% RH and 23°C. For the pulp fraction then, the basis weight includes 5-7% of moisture. Raw materials are only a part of total cost. This part is determined solely by the net use of each material per unit of product.

Fixed costs are incurred on a time basis. The time basis is the Nominally Available Hours of Production (**NAHP**). The fixed parts of the total cost relate to capital, operations apart from raw materials, and labor. All these costs, except some of those for steam, power, etc. are incurred on a time basis.

M = Maximum production, tons/hour. This is the nominal rate of production when everything is working as it should and the machine is operating in favorable ranges of basis weight, speed, etc.

C =	Total Capital Costs / NAHP.	(36)
L =	Total man-hours / ton at NAHP x Cost / man-hour x M	(37)

Note that C and L should include <u>all</u> capital and labor costs associated with the whole chain of production, i.e. including everything from the Forest and/or Receiving through Engineering, Maintenance, Administration, Warehousing, and Inventory.

 $\mathbf{F} = \mathbf{C} + \mathbf{L}$. Fixed cost per **NAHP**

acceptable product is produced or not.

V = Variable costs / ton run on the PM excluding raw materials costs. Expressed as cost / ton run across any part of the paper machine. These costs include steam and power costs, refining, vacuum, air, hydraulics, control, etc. In reasonably normal operation these costs are constant

Then all fixed costs are summed up and spread on the theoretical maximum number of tons, M, i.e. Fixed cost per ton product = F / M.

as soon as there is furnish on the wire(s) and, unfortunately, independent of whether an

In practice there are many causes of lost time, occasionally due even to lack of orders, and there are many losses that should not always be considered as broke. Trim losses in making cut sheet products is one example. Nevertheless, in order to keep things simple and comparable from a technical point of view, all lost material is considered as broke and all lost time beyond **NAHP** as being connected to the production of broke. This general case is easily specialized when considering an individual mill or machine.

Variable costs per ton product, excluding raw materials = V. These are the nominal values at full and 100% efficient production, T. If the production is less than this number, say t tons, then the costs are accounted as follows. The fraction of time that broke is produced is assumed to be **all** the lost time. Hence, if the fraction of production that goes to broke is **B** then $t = T \cdot (1 - B)$.

Fixed cost per ton <u>accepted</u> product is $ca = F / t = F / [T \cdot (1 - B)]$. The extra capital cost per ton <u>accepted</u> product is the Capital Cost of Broke, CCB = ca - F / T, so

$$\mathbf{CCB} = [\mathbf{F} / \mathbf{T}] \bullet [\mathbf{B} / (1 - \mathbf{B})]. \tag{39}$$

It tends to zero as it should when the broke fraction, **B**, approaches zero. If half of the production run across the machine goes to broke ($\mathbf{B} = 0.5$) then the extra capital cost of broke equals the nominal total capital cost.

Variable cost per ton accepted product is va.

$$\mathbf{va} = \mathbf{V} \cdot (\mathbf{T} / \mathbf{t}) = \mathbf{V} / (1 - \mathbf{B})$$
(40)

The extra variable cost per ton accepted product is the Variable Cost of Broke, VCB

$$\mathbf{VCB} = \mathbf{V} \bullet [\mathbf{B} / (1 - \mathbf{B})]. \tag{41}$$

(38)

CODA

All the necessary pieces are presented above. They make it possible to build computer programs with which all elastic and optical properties of even the most complex paper, board, and composite sheet products can be computed. Also required, of course, is a data base covering materials of interest. Expansion of the basics into the realm of strength properties, surface smoothness, air permeability, etc. seems to be feasible. It is feasible to include formulas connecting various processing variables, such as press and calender loads, and processing measures, such as freeness or Schopper-Riegler, and to connect them to product properties. This is most conveniently done through the intermediary variables density and volume concentration.

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- H. J. Schaffrath und L. Göttsching: Das Papier 1992, Heft 10A, p. V74 V76. Their curves are turned upside down compared to Figure 6 and show <u>stress</u> as a function of linear strain.

Transcription of Discussion

Some Fundamentals of Paper and Board Engineering

Professor Douglas Wahren, The Paper Professor AB

Peter Wrist, Consultant, Peter E Wrist, USA

Your formulations are very effective apparently in helping you predict the properties of the sheet. Ultimately of course we are concerned with the properties of the product as the customer will use it. Do you have any thought as to how you can better translate the customers requirements into the sheet characteristics which your formulation calculates? Many of our sheet property specifications do not relate very well to the customers use requirements and this leads to significant over-design in the paper requirements, adding significantly to the cost of the furnish. If we truly want to minimise cost of the paper we need a better way of translating the critical properties specific to a customers intended use into paper sheet specifications.

Douglas Wahren

If you can transmit the customer's requirements on the sheet to those involved in product design and development, you can do many things. For instance you can test print them in the computer and check some critical parameters. The real trick is to get feedback from the customer to the right people in the mill - once you do that I think we can work out some answers. It is very important to have sufficient knowledge of the customer's process and of his customers' requirements to avoid 'overdesign' and unnecessary costs.

Ilkka Kartovaara, R&D Vice President, Enso Group, Finland

I think a very central issue here is when are the volumes additives and when are they not. We know very well that in pigment mixtures they are not because of different degrees of packing. For the filler you have had to use a different form of mixing rule than for the fibres. My question is can you really put this situation in these two distinct categories, in the one category where the volumes are additive and the other category when the total volume is not increased at all.

Douglas Wahren

I think I understand your question. I have tried to answer it in practice. The answer is yes it is possible to classify materials and set limits to how they mix. The limits are given by, on the one hand that you can assume that the volumes are additive. Then the density

will usually change. At the other end of the spectrum you can assume that the volume concentration is unchanged. The differences of the final outcomes are not large. There are effects which have to be validated by experiments. I did not say that you can eliminate more than 90% of the laboratory work; you have to get calibrated ie you have got to make some mixtures and check them out.

Dr Derek Page, IPST, USA

My understanding of what you are saying is that the whole question of making paper is so complex and so confusing that most of the advances in paper physics that have been made in understanding have to be set aside and you have to start again using very simple empirical relationships when it comes to designing a sheet of paper from scratch. Is that a fair statement?

Douglas Wahren

That is a fair statement of the way I have attacked it in order to be able to do it at all. I have tried to structure these formulas, simple power functions, to be consistent with the results of more detailed network calculations. Within bounds they are well and much more easily described by simple power functions, and experimental measures of the exponent. That's all one needs actually.

John Waterhouse, Senior Associate Scientist, IPST, USA

At which point do you begin to model the economics because obviously you have got the bounds of the physical properties, do you do that first and then later bring in the economics of the situation.

Douglas Wahren

Very good questions. The answer is yes depending on the situation. If I am working with an operating mill which has a problem, and what they need is optimisation of their return on investment, then I try to model the problem as is and take the specifications, eg bending stiffness, to be above a certain limit, and the density of the top layer has to be above a certain limit to provide a smooth enough surface - those are physical constraints. The model is then hidden below an Excel calculating sheet where the economics are shown. For someone who works on designing better sheets, less costly pulp mixes and so on, the sheet design comes first and economics may be introduced at any time. *Professor Jacques Silvy, Universidade da Beria Interior, Portugal*

Thank you very much for this very nice approach on the physical properties. I think you point out an extremely important thing. We build the paper in volume, we do a sheet but we need caliper and your selection of the volume as a main parameter is a very clear demonstration of this. We have to transform it in terms of density, in a general point of view because we sell the paper by weight but we must have in mind that we construct first a structure and we need volume. One point more when you speak of the mean free path of photon and you said it is linked with the scattering coefficient: clearly it is an inverse relation. We did that in 1961 in a corpuscular approach of the theory of light diffusion. We were mixing in terms of length and not in terms of weight.

Douglas Wahren

That is correct. I should have expressed it more clearly.