Corrosion of Electrostatic Precipitators

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Corrosion problems in electrostatic precipitators are reviewed. Acid dewpoint corrosion is the major cause of corrosion. The operating variables which influence corrosion and some general means for reducing corrosion rates are described.

Introduction

Electrostatic precipitators require expensive maintenance because of corrosion. These corrosion problems have been surveyed by TAPPI and summarized by Henderson (1). The TAPPI survey identified four 'major' areas of corrosion: sidewalls at vertical corners, outlet vanes and outlet area, ductwork and sidewall access doors. 'Limited' areas of corrosion included wire weight guide frames, sidewalls, inlet vanes and inlet area, instrument penetrations, dry drag scrapers/dry bottom pan area, wet/dry cross conveyors, wet bottom pan area, and steel stacks. Figure 1 illustrates some locations of corrosion.

The principal cause of corrosion in precipitators is dewpoint corrosion. This form of corrosion involves the condensation of acid vapors, primarily sulfuric acid, onto structural surfaces and consequent attack of the material. The acids condense if the temperature falls below their dewpoints.
The acid dewpoint corrosion of electrostatic precipitators is not thoroughly understood. Most of the present knowledge has been gained from studies of power boiler precipitators, and further work is required for recovery boilers. In the meantime, the application of present understanding to precipitator corrosion problems should indicate some areas for improvement and may reduce significantly the costs of maintenance.

**Flue gas composition**

Sulfur dioxide (SO₂) and sulfur trioxide (SO₃) are produced during combustion of kraft liquor in the recovery boiler. The formation of sulfuric acid (H₂SO₄) depends on the equilibrium between sulfur trioxide, water vapor and H₂SO₄ in the flue gas:

\[ \text{SO}_3 + \text{H}_2\text{O} = \text{H}_2\text{SO}_4 \]

Below the dewpoint the acid will condense. Higher dewpoints caused by increased levels of H₂SO₄ can spell trouble because acid can then condense at higher temperatures, which would be obtained more easily in operation.

The acid dewpoint temperature is higher than the water dewpoint. At temperatures between the sulfuric acid dewpoint and the water dewpoint, hydrochloric acid vapors (HCl) also may condense from the flue gas. The hydrochloric acid could originate from the chlorides in the recovery boiler. Halstead and Raask (2) found, for coal-fired boilers, that all NaCl present in the coal was vaporized in the combustion chamber. Some of the NaCl would then react with sulfur dioxide and water via

\[ 2 \text{NaCl(g)} + \text{H}_2\text{O} + \text{SO}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{Na}_2\text{SO}_4(g) + 2 \text{HCl} \]
Condensation of hydrochloric acid may accelerate corrosion at lower temperatures. At still lower temperatures, water condensation can cause 'sweating' and widespread corrosion.

Flue gases containing high levels of $\text{H}_2\text{SO}_4$ have higher dewpoint temperatures, thereby increasing the chance of corrosion. Higher $\text{SO}_3$ and $\text{H}_2\text{O}$ concentrations will form more $\text{H}_2\text{SO}_4$ and therefore raise the dewpoint. The dewpoint temperature is related to the pressures of $\text{H}_2\text{O}$ and $\text{SO}_3$ (or $\text{H}_2\text{SO}_4$) via the Verhoff-Banchero equation (3-5). McDonald and Dean (6) have presented graphs of dewpoints and condensate composition for vapor mixtures of $\text{H}_2\text{O}$ and $\text{H}_2\text{SO}_4$. If a surface is maintained at a temperature lower than the acid dewpoint but higher than the water dewpoint, the concentration of acid condensate which forms can be predicted using these graphs if the water vapor content of the flue gas is known (6). The acid concentration of the condensate will be decreased as the dewpoint is decreased (7). Thus, at lower temperatures, water is present in the condensate and the combination of acid and water can make salt cake deposits sticky and more corrosive.

The $\text{SO}_3$ composition and consequently the $\text{H}_2\text{SO}_4$ concentration is affected by furnace firing temperature, fuel-air ratio, primary-secondary air ratios, and furnace bed temperature and configuration (3). A high level of excess air increases heat losses and favors formation of $\text{SO}_3$ and sulfuric acid (8). Higher $\text{SO}_3$ levels also may result from higher sulfidity. There is a need to define optimum conditions for control of corrosion within the constraints of efficient recovery boiler operation.

Higher moisture content in the flue gas can raise the dewpoint. A major source of moisture in the precipitator is steam used for sootblowing. Dewpoint
can be raised locally by moisture introduced by air leakage into the precipitator. These air leaks also lower the temperature below the dewpoint. Air leakage and low temperature were undoubtedly factors in the corrosion of the access door shown in Fig. 2. Moisture from the wet bottom of precipitators also may raise the dewpoint near the bottom. Figure 3 illustrates corrosion at the liquid/gas interface of a baffle plate in a wet bottom precipitator.

Figures 2 and 3 here.

The amount of hydrochloric acid in the flue gas can affect the corrosion rate, depending on the temperature. Kear (9) found that above the $\text{H}_2\text{SO}_4$ acid dewpoint temperature the addition of $\text{HCl}$ gas did not appear to increase corrosion but between the water and acid dewpoints, addition of $\text{HCl}$ gas (0.015%) increased corrosion by some 40%. Below the water dewpoint temperature ($40^\circ\text{C}$) a very large increase in corrosion was observed, and this was greatly accelerated by the addition of hydrochloric acid gas. In coal-fired power stations, $\text{HCl}$ concentration in the flue gas has been found to be directly proportional to the chloride content of the coal (10). A similar effect would be anticipated for pulp mill recovery boilers; $\text{HCl}$ concentrations would be reduced if chloride concentrations in the recovery boiler were lowered.

Temperature

The temperature must be maintained above the acid dewpoint to prevent condensation of acids. The TAPPI survey (11) of NCE electrostatic precipitators found that those units with no corrosion averaged a test temperature of $384^\circ\text{F}$ and those with a serious problem averaged a test temperature of $361^\circ\text{F}$. Although flue gas temperature did not correlate very well with corrosion, if the units
were grouped by age, sulfidity and shell arrangement, a weak correlation with flue gas temperature was seen (12). Other factors apparently exert a strong influence.

Maximum corrosion rates would be experienced at temperatures below the dewpoint. The corrosion rate is governed by the rate of acid deposition and not by the rate of reaction between metal and acid. In laboratory experiments, Flint and Kear (13) found that for a surface of given temperature, more acid was deposited from gases of higher dewpoint. They also found that, irrespective of the dewpoint temperature, the rate of corrosion reaches a maximum at a surface temperature of the steel 20–45°C below the dewpoint and this corresponds with the maximum rate of condensation. The maximum corrosion rate does not occur at the dewpoint because apparently there is less acid present at that temperature. Furthermore, they found that the concentration of condensed acid changed little with surface temperature even though the amount of condensation varied. Thus, surface temperature and dewpoint temperature are the two factors of major importance in determining acid concentration.

Flue gas temperature is influenced by feedwater temperature, economizer cleanliness and boiler load (1). Temperatures would be lower during periods of low boiler load. During startup and shutdown, temperature cycling would be expected and acid deposition could occur. Temperatures may be increased by changing water flows and boiler load. It is desirable to maintain the flue gas temperature 50°F above the dewpoint to allow for partial load operating conditions and low temperature areas in the precipitator (3). Several means are available for doing this. Flue gas temperature may be increased by removal of tubes from the cascade evaporator or installation of a bypass duct around the cascade evaporator (3). This change could help maintain temperatures above the
dewpoint, but a penalty would be paid in heat loss. Monitoring of temperature could be performed to detect excursions of temperature which are common even under steady-state operating conditions (14). Prevention of localized areas of low temperature would also be helpful.

Poor flue gas distribution and local areas of low flue gas temperature or surface temperature will compound difficulties with low temperature resulting from upset conditions or operating difficulties. High corrosion rates can be encountered in localized areas of low temperature known as 'cold spots'. These cold spots may be caused by poor insulation, air in-leakage or poor air distribution in the heated shell. For example, poor insulation and air in-leakage stimulate corrosion of side wall access doors as illustrated in Fig. 2. Air leakage also can occur at test ports, expansion joints, damper seals, flue and precipitator connections and rapper rods (3). Poor insulation and low flue gas temperatures are associated with stack corrosion problems (1). The TAPPI survey indicated that temperature of the heated shell of the precipitator can influence corrosion of sidewalls (1,12). The TAPPI survey (1) also reported a study by Wheelabrator-Frye which showed that significantly lower temperatures occurred in the bottom area. Without the heated shell in operation, the bottom sidewall temperature was 50°F lower than the inlet gas temperature. Design of heat jackets should include dampers to adjust the gas flow distribution of heated air. Problems with these systems are often the result of improper system operation and maintenance and high heat consumption. Another source (15) reported temperature drops across their precipitator of 32°F. The flue gas was colder across the bottom, across the top in the corners, and against the top and bottom of the division wall which separated one side of the precipitator from the other. These problems may also have been related to poor flue gas distribution.
Caron cited inlet gas distribution as a problem (16). The lower portions of the collector plates, especially toward the gas outlet of the precipitator (where the flue gas is cooler), become sensitive to temperature variations (15,17). Figure 4 illustrates an example of corrosion at the bottom of a collector plate. Cold spots in the precipitator may be eliminated by improving flue gas flow distribution.

Figure 4 here

Velocity

Low velocity of flue gases in the precipitator can lead to the formation of salt cake buildups. These hygroscopic salts can then absorb moisture and locally raise the dewpoint. They may also provide a poultice under which localized attack could take place. Corrosion of ductwork occurs in areas of salt cake buildup and may be associated with inadequate flue gas velocities (1). The buildups may also indicate low temperature, low velocity or localized high dewpoint (perhaps due to air in-leakage).

Low flue gas velocity may also result in poor circulation or distribution of flue gases which will contribute to formation of cold spots. If the velocity is less than 0.7 m/s, corrosion can be a problem (1). Volume oversizing can lead to low gas velocities and dust buildup on the turning vanes and excessive buildup in the inlet nozzle (1). Maximum rated flue gas velocities should be used. Design flue gas temperatures should be reviewed or adjusted upward to minimize the actual low load operating flue gas temperature (1).
Salt cake composition

Corrosive species contained in the salt cake may accelerate corrosion in the presence of acid. For example, the sulfuric acid may react with chlorides in the salt cake to form hydrochloric acid. The salt cake and the acid itself are hygroscopic and may absorb moisture if cooled, leading to formation of a salt-cake poultice. On the other hand, the salt cake may neutralize small amounts of acid. McDonald and Dean (6) performed corrosion tests which indicated that basic fly ash (power boiler) neutralized a major portion of the acid as it condensed but that this effect was limited to a surface layer. A layer of CaSO₄ then formed and prevented the underlying soluble base from being utilized. In tests with a condenser in a stack, Piper and VanVliet (18) observed that deposits were dry in appearance above 150°F. As the temperature was reduced, they became more sticky and moist. At 105°F, the deposit consisted of nearly equal parts of solid and liquid and was sufficiently liquid to flow. Thus, corrosion may be increased by corrosive species in the salt cake and by the absorption of moisture.

There is some evidence that corrosion deposits can enhance further corrosion. The role of FeSO₄·H₂O in dewpoint corrosion has been studied by Dawson et al. (14). They found that the passivation by FeSO₄ was not maintained under thin film conditions expected for condensation. The corrosion rate increased after 5-12 hours, and visual examination suggested that the sulfuric acid was becoming diluted because of water absorption. They noted that FeSO₄ may be hydrated with 1, 4, or 7 H₂O molecules, depending on the humidity. When the water vapor pressure exceeds the standard vapor pressure of FeSO₄·7H₂O, the salt will form a solution in equilibrium with the water vapor pressure. In tests with FeSO₄ crystals, passivation was accompanied by drying out of the surface,
followed by hygroscopic absorption of water and flooding of the surface. They noted that this phenomenon was similar to the sweating which is observed in plants after shutdown.

**Construction materials**

Stainless steel has been found effective in reducing corrosion on wet bottom pan sides (1). In gases, however, the stainless steel may offer no advantage (18). The high price of stainless steel limits its use to areas of severe corrosivity or for critical parts. It may be affected by stress corrosion cracking if chlorides are present in sufficient concentrations.

Various coatings may be used to reduce corrosion rate. Organic coatings such as vinyl ester coatings may be applied around areas of air in-leakage (19). Cox et al. (20) found that in laboratory tests in flue gas environments and service trials in coal-fired power stations, fluoroelastomer copolymer showed the greatest resistance in the acid dewpoint range (210-275°F). An isocyanate-cured pitch epoxy and a polyester showed promise. These coatings were superior to PVDF, PTFE loaded polyamides and chlororubbers. In other tests, in flue-gas-desulfurizer environments, White and Leidheiser (21) found that vinyl ester, fluoropolymer and some epoxies performed well in H₂SO₄ solutions but that polyester was attacked.

Inorganic coatings were investigated by Piper and VanVliet (18). Nickel-phosphorus, fired under reducing conditions, was the best coating, followed by crack-free chrome plate, nickel-phosphorus applied by a wet reduction process and sprayed aluminum. Cox et al. (20) found that arc-sprayed aluminum, an experimental TiO₂ coating and enamels were resistant to flue gas (to 135°C), but flame sprayed oxide coatings were unsatisfactory.
Fiberglass reinforced composites have been found to perform satisfactorily up to 300-350°F in recovery boiler electrostatic precipitator ducts (18,22,23). Some elastomeric materials for expansion joints have been found to resist operating temperatures up to 400°F in flue gas stack systems (24).

Conclusions

Acid dewpoint corrosion involving sulfuric and hydrochloric acids is the main cause of corrosion in electrostatic precipitators. Flue gas composition, temperature, velocity and salt cake composition all influence the corrosion process. This review of corrosion in electrostatic precipitators indicates that some simple remedies for corrosion are available. Application of these could lead to improved operation and reduced maintenance.

Acknowledgment

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Figure 1. Corrosion problem areas in an electrostatic precipitator.
Figure 2. Corrosion of an access door.
Corrosion at the liquid/gas interface of a baffle plate in a wet bottom precipitator.
Figure 4. Corrosion at the bottom of a collector plate.
SIMULATION OF PRODUCT QUALITY AND PROCESS PERFORMANCE

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Simulation of Product Quality and Process Performance

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ABSTRACT

In conventional flow sheet simulation, the main results are flows of material and energy throughout the process. The performance of the process is derived from these flows and through process economics, yields, purities, etc. Development of a simulation is possible because the simulation variables are invariably conserved quantities. However, factors such as product quality have far greater economic impact and yet are far more difficult to predict.

The reason that these features are generally not present in flow sheet simulation packages is that performance attributes or PATs usually depend on non-conserved quantities. In some cases PATs can be predicted by quantitative models involving nonconserved and conserved variables. Predicting these is difficult but feasible with conventional simulation. Often PATs depend on sequences of events best described by qualitative information, i.e., heuristics, which are best handled by expert or database management systems. Simulation of PATs in general requires techniques for modeling, mixing, splitting and converting nonconservative quantities and ways of expressing events, sequences and other qualitative information. This suggests that a combination of conventional simulation and an expert system is needed.

This paper discusses concepts for modeling and simulation of PATs in the conventional simulation environment. New ideas of relating information in the simulator with the qualitative information in the expert system are explored. Simulation of a mechanical pulping process for papermaking using the MAPPS simulator is used for illustration.

INTRODUCTION

No one would argue that the rate of growth of information has accelerated rapidly in the past 50 years. The computer has provided a powerful means of capturing, processing, and analyzing this information and knowledge. In the chemical engineering field, process simulation was developed from the fundamental need to automate the analysis of larger and more complex problems with greater speed and reliability. Engineering-oriented process simulators such as ASPEN and FLOWTRAN were developed to compute mass and energy balances in the petrochemical industry (Evans et al. 1977, Evans 1978, Westerberg 1979, Evans et al. 1979, Seader et al. 1974, Rosen et al. 1977). These simulators contain a library of mainly general-purpose unit operations. These provide detailed mass and energy balance calculations of interest to the pulp and paper technologist.

Whether simulators are steady state or dynamic, they are generally built from building blocks which model each specific unit operation in the flow sheet. The modular construction provides a completely general and flexible method of simulating virtually any process in principle. Discounting the aspects of time and assuming the process to be deterministic rather than stochastic, process simulation may be viewed as existing in at least two dimensions as shown in Fig. 1. The horizontal dimension represents the breadth, i.e., number and level of detail, of process modules in the library of the simulator. The vertical axis represents the depth of detail within each module and within the stream structure of the simulator to represent detailed aspects of each process step. Initially the main emphasis is to develop sufficient breadth to handle most processes. Depth was developed to the extent that mass and energy balances are computed; most physical and chemical components are described and yields are computed accurately.

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<td>D Process models ————&gt;</td>
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<td>P Built-in stream structures</td>
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<td>T Flexible stream structures</td>
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<td>H Physical property models, databases</td>
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Figure 1. Overview of steady-state process simulation.

At a still greater depth, physical property databases and models enable detailed calculations of phase behavior, transport processes, and detailed physical phenomena. Processes simulators such as ASPEN and MAPPS are capable of simulating complex slurries consisting of gases, liquid, and solid phases. The complex liquid phase consists of dissolved components such as electrolytes. The solid phase consists of suspended solids and fibrous components.
At a still deeper level, the most advanced process simulators such as ASPEN provide for characterization of the component attributes such as chemical composition and the substream phase attributes such as particle size distributions. Coupling between particle size and composition can also be accounted for through a stream attribute matrix. This enables very detailed calculations to be made on combustion, separations and mixing of solid components (Jones 1984). This increasing level of detail is more urgently needed to provide the detailed data to make these tools useful to chemical process industries.

The conventional process simulator provides information in three main areas: flows of mass and energy, processing conditions, and economics. The primary uses of conventional simulation are for design, optimization, and decision-making. Decisions which rely on simulation input could range from day-to-day operations such as determining the boil-out schedule for a complex system of evaporators to the synthesis of process improvements for mechanical pulping processes to produce pulp for newsprint (Venkatesh 1976).

Yet it is not difficult to imagine how much more significant this information would be if it also included a measure of process performance, product quality, and product properties. Information of this type is vital to the survival and growth of business in the future. However, current process simulators do not yet provide the still greater level of detail required to predict this important information.

One reason for this seemingly obvious oversight is that the relationships between fundamental variables and observed or measured properties and product quality is often ambiguous and qualitative rather than deterministic and quantitative. However, a more common reason is that this information is very dispersed and has not yet been put in the form of models or tables of data which can be readily processed by a computer. This paper describes the techniques now being used to develop a capability to predict product quality and process performance in MAPPS, a sequential, modular, steady-state simulator, developed at The Institute of Paper Chemistry.

SYNTHESIS OF HEURISTIC AND QUANTITATIVE INFORMATION

A great deal of both qualitative and quantitative information exists relating fundamental variables with process performance and product quality. This is particularly true in the pulp and paper industry, which is the objective of MAPPS simulation. The quantitative information is of the type from which mathematical models can be constructed. Qualitative information and relationships, on the other hand, can be readily codified in the form of tree structures. Trees are related to "linked lists" or "graphs" in which the nodes of each branch provide the information on the connectivity of the tree. The rules containing knowledge base of many expert systems are based on a tree structure. The inference engine accesses and manipulates the rules to provide the "answers" or to reach specific goals. Expert systems have been the source of much debate and discussion. G. Stephanopoulos has summarized many of the issues well in a recent article (Stephanopoulos 1986). An example of a simple tree structure to store qualitative information on a paper process is shown in Fig. 2. The nodes describe major steps in the manufacture and processing of pulp and paper. At the root level is the tree species. At the next level is the growth pattern, i.e., summer- or springwoods. Next is the general pulping process categorized by overall yield of wood. At a still deeper level, the process is specified, i.e., kraft, sulfite, mechanical, etc. Following this, the general fiber pretreatment conditions are specified. This is followed by the bleaching conditions and so on. The tree structure is the logical basis for the queries to the user. The user responses in turn generate a list containing flags whose values determine the qualitative nature of the process conditions. An example of the process flag list or PFL is shown in Fig. 3.

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The PFL provides the next level of depth for the process as shown in Fig. 1. The information in the PFL list is used to specify parameters used by the higher level process models in their calculations. These parameters represent the lumping of many factors in the process models to account for such things as species variations, equipment design, and processing conditions.

As an alternative, the expert system can be used to bracket values of selected paper properties based on the knowledge base and inferencing system. This
The technique can work if the goals associated with different branching through the tree are ranges of physical property values. The user could add rules to the knowledge base to make this approach more meaningful.

**PERFORMANCE ATTRIBUTES**

The process models in MAPPS not only calculate mass and energy flows, they now contain the additional detail to compute the fundamental performance attributes which are used by the product quality models (see Fig. 1). The PATs can have a variety of structures, but the most convenient form is to pattern them after the stream structures themselves. Thus, the PATs are lists of variables relevant to each physical stream in MAPPS. The example PAT structure shown in the lower portion of Fig. 4 contains the following information: tags to the corresponding physical stream, tags to the PAT structure, a key composition variable relating to yield, variables representing the fiber morphology such as the average fiber length and width, fiber length distribution standard deviation and width distribution standard deviation, specific surface area parameter, a variable relating to bleachability, i.e., absorption coefficient, followed by several variables representing intrinsic fiber attributes such as fiber specific gravity, tensile strength, cell wall thickness, and modulus.

- **Stream ID**
- **Type**
- **Thermodynamic data**
- **Phase data**
- **Total flow**
- **Component flows**
- **Performance Substream Type**
- **Yield parameter**
- **PATs Fiber morphology parameters**
  - Length, a_l
  - Width, w
  - Surface area development parameter
  - Curl parameter
  - Absorption coefficient
  - Average fiber physical property
    - Density
    - Tensile strength
    - Modulus

**APPLICATION TO A MECHANICAL PULPING SYSTEM**

The concepts described above are now applied to the simulation of a complex mechanical pulping system shown schematically in Fig. 6 and in MAPPS block form in Fig. 7.

The process can be broken down into the following process steps: refining, mixing, splitting or fractionation, fiber concentration control (i.e., consistency control), and bleaching. Fractionation steps are made up of a series of screens or centrifugal cleaners, i.e., hydrocyclones.

Energy is supplied to the refiners to rotate the patterned plates which shear the fiber bundles causing the fibers to separate. Fibers are reduced in length and width and the distributions of fiber length and width are changed. Fiber impacts lead to fibrillation of the fiber surfaces leading to a great increase in surface area of the fibers. Screening preferentially separates out long fibers from short fibers. Centrifugal cleaning separates dirt and more spherical fibers, i.e., those with low length to width ratios. During bleaching, chemical oxidation of color bodies in the fibers reduces light absorption and brightens the fibers. Stocks are mixed for recycle control and to dilute the stock. Stock mix tanks also store the fibers to disentangle the fiber bundles and relax residual stresses in the fiber structures.

**Figure 4. MAPPS stream and substream structure.**

**Figure 5. Overview of quality and performance calculations with MAPPS.**

**PERFORMANCE AND QUALITY MODELING**

The performance and quality modules or PPM's can be placed anywhere in the flow sheet to show the development of properties throughout the system. The differences in property values across operation modules represent a measure of performance of that processing step. Process performance can be calculated as the relative differences in selected properties in various ways, for example, for a change in processing conditions or for fixed processing conditions for different operations which perform the same basic task. For example, the contribution of different screening and cleaning designs can be compared to select the best system among various candidates. The processing conditions can also be determined so as to optimize process performance or in conjunction with other modules to maximize specific final properties of the paper.
Every process step has a direct or indirect effect on the PAT's values. The main feature of bleaching is the reduction of one of the key PATs: the absorption coefficient. The refining process reduces PAT's length and width and changes the standard deviations of each of the distributions. Refining also changes the surface area development parameter. Mixing of fibers tends to blend PATs based on relative mass flow of each stream. Fiber fractionation tends to produce streams with PATs greater or less than the entering fiber stream.

Refining energy converts chips into a distribution of fibers with a variety of lengths and widths. The average chip length and width is converted into a log-normal distribution of lengths and widths as shown in Fig. 8. In the secondary refiners, the entering fiber length and width distributions are converted to outlet distributions. The PATs representing the mean and standard deviation of each distribution are changed and stored in the PAT substream of the exiting pulp stream. The cumulative distribution functions are determined from the distribution statistics in the following fashion.

\[ XC_i = \frac{1}{2} \left[ 1 + \text{erf}(ZL_i) \right] \quad (1) \]

where

\[ ZL_i = \frac{[\ln(L_i) - \ln(L_g)]/\ln(a_g)/\sqrt{2}} \quad (2) \]

The weight fractions of fibers with lengths between \( L_i \) and \( L_i+1 \) is \( DL_i \).

\[ DL_i = XC_{i+1} - XC_i \quad (3) \]

\( DL_i \) is the discrete density function for length.

\( L_g \) is the geometric mean fiber length defined in terms of weight-average length and standard deviation,

\[ L_g = L \exp \left( -\frac{3}{2} \frac{\ln^2(\sigma_g)}{} \right) \quad (4) \]

The cumulative width distribution for each fiber stream is determined from the number-average width,

\[ WC_j = \frac{1}{2} \left[ 1 + \text{erf}(ZW_j) \right] \quad (5) \]

where

\[ ZW_j = \frac{[\ln(W_j) - \ln(W_g)]/\ln(a_g)/\sqrt{2}} \quad (6) \]

The weight fractions of fibers with widths between \( W_j \) and \( W_j+1 \) is \( DW_j \).

\[ DW_j = WC_{j+1} - WC_j \quad (7) \]

\( DW_j \) is the discrete density function for width.
and $W_{ng}$ is the number-average geometric mean width.

$$W_{ng} = W \exp \left(-\frac{1}{2} \ln^2(W)\right)$$

and

$$DW_j = WC_{j+1} - WC_j$$

is the discrete width density function.

The discrete density functions, $DL$ and $DW$ are used to determine the weight fraction of fibers in each length and width range. The joint probability that a fiber has length $L$ and width $W$ is given by the vector product of $DL$ and $DW$. The elements of the joint probability matrix, $C$, represent each unique combination of length and width. The matrix representation internal to each module is converted to the actual fiber categories in the pulp stream by the mapping shown in Fig. 9.

The process of mixing the components in fiber stock streams is straightforward. However, mixing of the PATs requires some discussion. The concepts are illustrated in Fig. 10. The joint probability matrix for each entering stock stream is generated by the method described above. The mixture $\mathbf{C}$ is the weighted average $\mathbf{C}$. The sum of the columns of the mixture $\mathbf{C}$ determines $DL$. The mean and standard deviation PAT values are determined from $DL$ and $DW$, respectively, and placed back in the PAT substream.

In bleaching, the fiber size distribution is not changed significantly. Bleaching is measured by the change in absorption coefficient, which is determined by integrating the reaction kinetics over the bleaching tower assuming plug flow, isothermal behavior. The calculated absorption coefficient is placed in the outlet PAT substream.

The total surface area development in the pulp, $SA$, is related to the fiber length distribution. Thus, it is influenced by energy input to the refiners, and mixing and splitting of the fiber streams. The specific surface area is found to be a function of the weighted-average of the log of the fiber length.
\[ W_{nj} = \frac{[\ln (W_j) - \ln (W_{nj2})] - \ln (\sigma_w)}{\sqrt{2} \ln (\sigma_w)} \]  

and \( W_{ng} \) is the number-average geometric mean width.

\[ W_{ng} = W \exp \left( -\frac{1}{2} \ln^{2}(\sigma_w) \right) \]

and

\[ D_{wj} = W_{cj+1} - W_{cj} \]

is the discrete width density function.

The discrete density functions, \( DL \) and \( DW \) are used to determine the weight fraction of fibers in each length and width range. The joint probability that a fiber has length \( L \) and width \( W \) is given by the vector product of \( DL \) and \( DW \). The elements of the joint probability matrix, \( C \), represent each unique category. The matrix representation internal to each module is converted to the actual fiber categories in the pulp stream by the mapping shown in Fig. 9. The process of mixing the components in fiber stock streams is straightforward. However, mixing of the PATs requires some discussion. The concepts are illustrated in Fig. 10. The joint probability matrix for each entering stock stream is generated by the method described above. The mixture \( C \) is the weighted average \( C \). The sum of the columns of the mixture \( C \) determines \( DL \), while the sum of the rows of the mixture \( C \) determines \( DW \). The mean and standard deviation PAT values are determined from \( DL \) and \( DW \), respectively, and placed back in the PAT substream.

Fiber fractionation is shown in Fig. 11. \( C \) of the entering fiber stream is determined in the usual fashion. An efficiency model specific to the screen or centricleaner determines the probability \( P \) matrix whose elements represent the probability that each fiber with length \( L \) and width \( W \) will flow to the rejects. The product of \( P \) and \( C \) defines \( C \) for the rejects. By mass conservation, the \( C \) for the accepts is obtained by difference. The mass flows of the components are determined by the mapping shown in Fig. 9. Before the PATs can be computed, the \( C \)'s are normalized to sum to one and the discrete length and width distributions, \( DL \) and \( DW \), are determined by summing over the columns and rows of each \( C \). The distribution statistics are then determined by the usual statistical rules and placed in the appropriate PAT substream.

In bleaching, the fiber size distribution is not changed significantly. Bleaching is measured by the change in absorption coefficient, which is determined by integrating the reaction kinetics over the bleaching tower assuming plug flow, isothermal behavior. The calculated absorption coefficient is placed in the outlet PAT substream. The total surface area development in the pulp, \( SA \), is related to the fiber length distribution. Thus, it is influenced by energy input to the refiners, and mixing and splitting of the fiber streams. The specific surface area is found to be a function of the weighted-average of the log of the fiber length.
where \( K \) is the surface area development parameter (Baldus 1977) which is a function of fiber concentration during refining (consistency) and specific power input. For secondary refiners, the outlet K-factor is a function of inlet K-factor, consistency, and specific power input. The formulas above enable computation of the change in the specific surface area across the refiner. The specific surface is strongly related to the drainage from the paper machine during forming, a key factor in the formation of paper.

Drainage rate is then computed from the appropriate performance model.

The various PATs plus the PFLs are then used to compute paper properties at selected points in the flow sheet. The properties are based on models most of which are currently under development. However, the present capabilities include predictions of handsheet bulk, tear, burst, tensile index, wet-web strength, and breaking length for unbleached pulp. For bleached pulp, the bleaching conditions stored in the PFL is combined with the properties of unbleached pulp to predict enhanced properties of the bleached pulp paper. These properties are density, surface roughness, tear, and other tensile properties.

A second type of information which can be generated by the expert system is a bracketing of the values of final paper properties. For example, a property such as tensile strength will have a maximum and minimum value regardless of the species, pulping technique, or paper manufacturing process, e.g., 0.1 g min to 100 g max. Species with long fibers tend to have high strength so the wide bracketing is narrowed to 50 g min to 100 g max for long fibers. If long fibers are produced by the kraft process, their maximum strength tends to be very high, 80 min to 100 max, while if produced by stone groundwood, strength tends to be lower. Thus, for long fiber, kraft strength is bracketed between 90 and 100 g while for stone groundwood, strength is bracketed between 50 and 60 g. However, if cooking conditions are excessive and yield is low, strength is reduced and the bracket is changed to 50 to 80 from 90 to 100 g.

The key is the development of rules which do not conflict and which can be applied in a general fashion regardless of other conditions. If there is a high degree of interaction between effects, then it may be very difficult to formulate sufficiently general rules for this application. The combination of specific models and brackets based on quantitative information from the process simulator and rule-based systems should provide great flexibility in obtaining an accurate if not a precise property prediction.

### OPTIMIZATION

The next major step in automating process calculations is the coupling of optimization with the process simulation. This coupling is currently under development with MAPPS. The objective function of most interest would be a combination of properties or process performance values predicted by the process simulator. The optimizer in conjunction with MAPPS would find the "best" processing conditions to maximize the objective function. The control variables would include processing conditions as well as process parameters in the PFL array. The starting point would be some feasible point defined by the user initially and converged by MAPPS. The converged simulation would automatically satisfy all the tear variables and in many cases implicitly satisfy many of the usual equality and inequality constraints associated with defining the optimum. These constraints are satisfied as MAPPS converges on the feasible solution. Other constraints not known a priori would be accounted for by the explicit optimization algorithm.

For the mechanical pulping system, the coupled MAPPS plus optimizer system is being used to predict the optimum feedstock, refining energy, and bleaching for maximum paper tensile, burst, and tear properties with minimal roughness. The results of this work will be available in the near future. Similar work of this nature has been reported previously (Venkatesh 1976).

### SUMMARY AND CONCLUSIONS

What has been described is a process simulation package which combines conventional process simulation of mass and energy balances with quantitative product quality models and heuristic process information analogous to an expert system format to generate a deeper level of simulation detail. The more fundamental PAT substream information forms the link between mass and energy balances and performance models to compute process and product quality and properties. The simulation is then coupled in a sequential and iterative fashion to a conventional optimizer to determine the processing conditions or process design changes needed to optimize product quality.

The combination of new features and expanded conventional features now being developed in MAPPS will provide a significant new tool for research, marketing and manufacturing in the pulp and paper industry. These techniques are equally applicable to the simulation of many other manufacturing processes where quality is of special significance.

### REFERENCES


**NOMENCLATURE**

- $\mathbb{C}$ Joint probability matrix
- $C_{ij}$ Element of C
- $\mathcal{DL}$ Probability density function - length
- $\mathcal{DL}_i$ Weight fraction fibers with average length, $L_i$ independent of width
- $\mathcal{DW}$ Probability density function - width
- $\mathbb{PAT}$ Vector or array of performance attributes
- $\mathbb{PFL}$ Process flag list