KCL-PAKKA: a tool for simulating paper properties

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ABSTRACT

A structural simulation method has been developed for the three-dimensional structure of paper. In the KCL-PAKKA simulation model, the porous sheet structure is compiled from fibers, fillers, and fines. Many paper properties can be calculated from the structure. A case study of copy paper shows how the simulation can be used to cut costs by finding the optimum combination of raw materials. A similar case study demonstrates an optimization for folding boxboard. The required paper or board properties are first specified, and the furnish mixture is then adjusted to minimize raw material costs.

Application:

Application: Structural simulation is effective in comparing paper properties and predicting costs. The new technique is much faster than traditional handsheet experiments.

The precise three dimensional geometry of the fiber network of paper is difficult to simulate. Our approach is to simplify the problem as much as possible, while still keeping the essential physical features of the fibers. These features include the dimensions of length, width, and diameter and properties such as stiffness (*1*, *2*).

Once these properties have been defined, a computer is used to simulate paper sheets for realistic furnish mixtures and to calculate the paper properties. The KCL-PAKKA simulation program runs on an ordinary workstation, requiring 10–20 Mb of working memory. The program generates a simulated sheet in a few minutes.

KCL-PAKKA SIMULATIONS

In the simulation, straight fibers are deposited on a square lattice one by one, as if they were settling out of a dilute suspension with no interactions. The fibers are placed and oriented on the lattice at random, as illustrated in **Fig. 1**. The program can also generate discretionary fiber orientations. Periodic boundary conditions are applied to fibers that cross the lattice boundaries.

The underlying lattice is divided into square cells with sides that are 10 µm long. This area is the in-plane resolution of the model. The length *L* and width *W* of individual fibers are integer multiples of the 10 µm unit length. Alternatively, a discretionary fiber width can be generated with the use of two unit widths. Usually the substrate consists of 1000 × 1000 cells, so the size of the model paper sheet is 1 cm². Sometimes we use smaller systems with fewer cells.

The nontrivial porous structure of real paper arises from the nonzero bending stiffness of fibers. The flexibility, T_f, of fibers is defined through a constraint on the height of "steps" that the fibers can form:

$$|z_i - z_j| / t_f \leq T_f \qquad (1)$$

where t_f is the fiber thickness and z_i and z_j are the elevations of the fiber at any two nearest neighbor cells *i* and *j* (**Fig. 2**).

High values of T_f give dense and well-bonded sheets, while low values of T_f lead to bulky and porous sheets. The bending rule (*1*) is a simplified version of the true bending equation that Görres *et al.* (*3*) employ in their analytical modeling of paper structure. The flexibility T_f can be related to the wet fiber flexibility *WFF* through Eq. 2 (*4*):

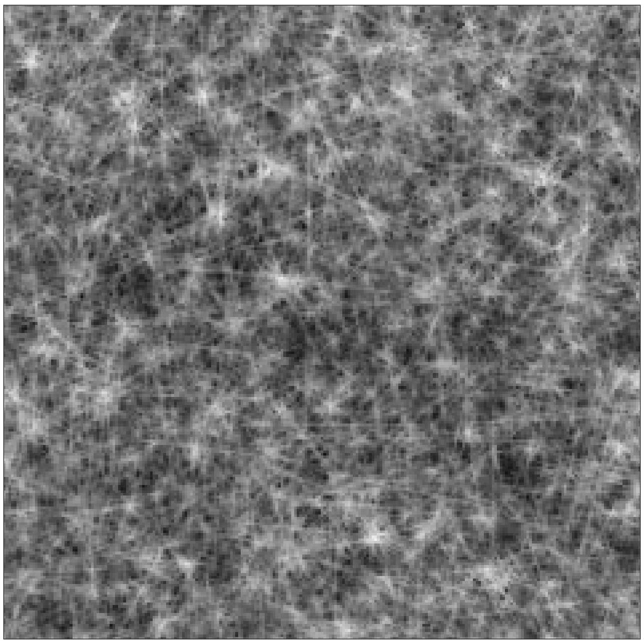
$$T_f = (C \times w_f \times WFF)^{1/4} \qquad (2)$$

where the constant $C = 5.4 \times 10^{-8}$ N·m depends on the wet pressing pressure.

We have fixed the value of *C* somewhat arbitrarily so that the simulated sheets roughly match handsheets in physical properties. It would be impractical to use measured *WFF* values directly because they are tedious to measure for each fiber fraction separately. However, measured *WFF* values serve to indicate the relative differences between furnishes.

In addition to the flexibility, properties assigned to the fibers include the dimensions (length, width, thickness), coarseness, and certain optical parameters, such as the refractive index. Papermaking pulps are modeled with three or four fiber fractions rather than with continuous distributions of the fiber dimensions. Usually these fractions are the long, medium, and short fibers, together with fines. Fines and fillers are described according to the same principles as fibers.

The KCL-PAKKA model does not take into account many aspects of real papermaking. The most important artifact is the surface roughness. Because the fibers deposit on a flat substrate lattice, the bottom side of the sheet becomes very smooth, much like a yankee dried paper surface. The top side resembles free-dried paper. We are working on a calendering mechanism that would let



1. Surface topography of a 45-g/m² sheet generated by the KCL-PAKKA model. [The sheet size is (0.7 cm)².]

	Mass fraction, %	Length, mm	Coarseness, mg/m	Wet flexibility, 10^9/N·m²
Aspen CTMP				
Long	3	1.9	0.275	5
Medium	47	1.7	0.173	15
Short	30	0.7	0.061	20
Fines	20	0.03	n/a	infinite
Pine kraft				
Long	30	4.0	0.386	30
Medium	40	2.5	0.227	50
Short	20	1.5	0.096	80
Fines	10	0.03	n/a	infinite
Birch kraft				
Long	10	1.8	0.207	100
Medium	40	1.2	0.151	150
Short	40	0.6	0.091	200
Fines	10	0.03	n/a	infinite

I. Properties of fiber fractions in the copy paper

us simulate the surface structures of the model sheets.

Despite all its simplifications, the KCL-PAKKA program simulates realistic paper properties for realistic furnish mixtures. From the network geometry, we can calculate the bulk, the optical properties, and the elastic properties of paper. Tensile strength and tear strength have been implemented only in a crude manner, and further development is still needed in that respect as well.

CASE 1: COPY PAPER

As an example of the potential of structural simulation, let us consider first the minimization of raw material costs of a copy paper. The optimization target was to minimize the raw material cost per ream (500 sheets) while keeping constant the bending stiffness (0.17 mN·m), the opacity (88%), and the brightness (Y-value = 89.8%). Tear strength was expected to be reasonable.

The main degree of freedom in the optimization was the replacement of hardwood kraft with aspen CTMP (**Table I**). This change leads to lower brightness and tear strength but to higher bending stiffness and opacity. This result allows a reduction in grammage. The loss of brightness was compensated for by adding filler.

KCL-PAKKA simulations were run at grammage intervals of 5 g/m² from 50 g/m² to 80 g/m². Of the total fiber furnish, a constant 30% was pine. CTMP percentages were 0%, 21%, 42%, or 63%, and the rest was birch kraft. The levels of filler content (in total ash) were 5%, 15%, and 25%. The filler was predominantly chalk, with the titanium dioxide percentages of 0%, 5%, 10%, and 30%. Thus, the total number of test points was 7 × 4 × 3 × 4 = 336. Five sheets per point were generated for statistically reliable results. **Table II** shows a sample of the simulation results.

For the cost optimization, the simulated values of stiffness, opacity, brightness, and tear strength were represented as polynomial functions of the CTMP fraction, titanium dioxide fraction, ash content, and grammage. The cost minimum was determined using these expressions, on the basis of the unit costs of the raw materials as given in **Table III**.

According to the simulations, the minimum cost per ream is obtained with a 68.1 g/m² sheet in which 60% of the birch kraft is replaced with aspen CTMP. The total ash is 14%, of which 30% is titanium dioxide. The raw material cost is 1.32 US$ per ream, which is 11% below the reference. Bending stiffness, tear strength, and brightness are the same as in the reference. Opacity is 89.9%, as opposed to 87.9% in the reference.

When calculated by the weight of paper, the raw material cost is 595 US$/metric ton in the reference and 620 US$/metric ton in the per ream optimum. The minimum cost per weight of paper would be given by a 80 g/m² sheet, where 9% of the birch is replaced with aspen CTMP and

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Boxboards, copying papers, costs, folding boards, models, packaging materials, paper properties, paper structure, simulation, test methods, three-dimensional design

the total ash content is 23%, of which 5% is titanium dioxide. The raw material cost would be 588 US$/metric ton. Tear strength would drop from 347 mN to 300 mN.

Calendering was ignored in this study of copy paper. One might argue that calendering would alter paper properties proportionately in the same way in all furnish mixtures. A primitive calendering mechanism is already incorporated in the KCL-PAKKA program. For demonstration purposes, we applied it to the reference and the simulated sheet which yielded the minimum cost per ream. **Figure 3** shows both the light scattering coefficient and the bending stiffness plotted against roughness.

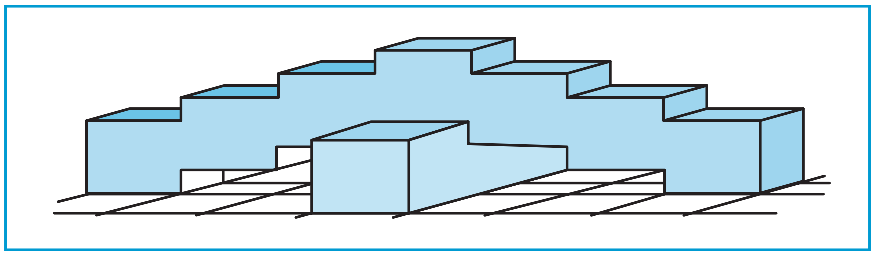
CASE 2: FOLDING BOXBOARD

In this case, we sought the minimum raw material cost by varying the relative grammage proportions of the middle and top plies and by varying the filler (talc) content of the top ply (**Table IV**). The optimization target was to minimize raw material costs per weight while keeping constant both the bending stiffness (at 29 mN·m) and the brightness (at a Y-value of 78%). The total grammage was kept constant at 280 g/m². The middle ply was entirely old newspaper.

A reduction in the grammage of the top ply reduces bending stiffness and brightness. The effect on bending stiffness can be compensated for by increasing the softwood content of the top ply, whereas the brightness reduction can be overcome by increasing the filler content.

KCL-PAKKA simulations were run for grammages in the top ply of 25, 35, and 45 g/m². The pine kraft content in the top ply was 20%, 40%, and 60%, and the rest was birch kraft. The level of talc filler (in total ash) was 5%, 10%, and 20%. The total number of simulation points was 27.

This optimization was run along the same lines as that for the study of copy paper. The optimum result was obtained for a top ply with a grammage of 34 g/m², with 8% ash and a pine kraft content of 60%. The raw material cost would be 425 US$/metric ton, which was 6.4% lower than the reference. In **Table V**, the properties of the boxboards for the two cases are compared.



2. Fiber bending in the KCL-PAKKA model. The height of the "steps" is $T_f = t_f/3$, where t_f is the fiber thickness. Fiber width w_f is equal to the size of the underlying cells.

Grammage, g/m²	Density, kg/m³	Bulk, cm³/g	Opacity, %	Y-value, %	Bending stiffness, mN·m	Tear strength, mN
50	694.8	1.44	78.7	89.8	0.04	286
55	698.3	1.43	80.8	89.8	0.05	315
60	701.5	1.43	82.6	89.8	0.06	343
65	704.5	1.42	84.1	89.8	0.08	371
70	706.7	1.42	85.5	89.8	0.11	400
75	709.1	1.41	86.8	89.8	0.14	428
80	710.9	1.41	87.9	89.8	0.17	456

II. KCL-PAKKA results in the reference case of 0% CTMP, 0% TiO_2, and 20% ash

Copy paper	
Pine kraft	700
Birch kraft	700
Aspen CTMP	450
Chalk	175
TiO_2	2200
Folding boxboard	
Pine kraft	700
Birch kraft	700
Old newspaper	350
Talc	175

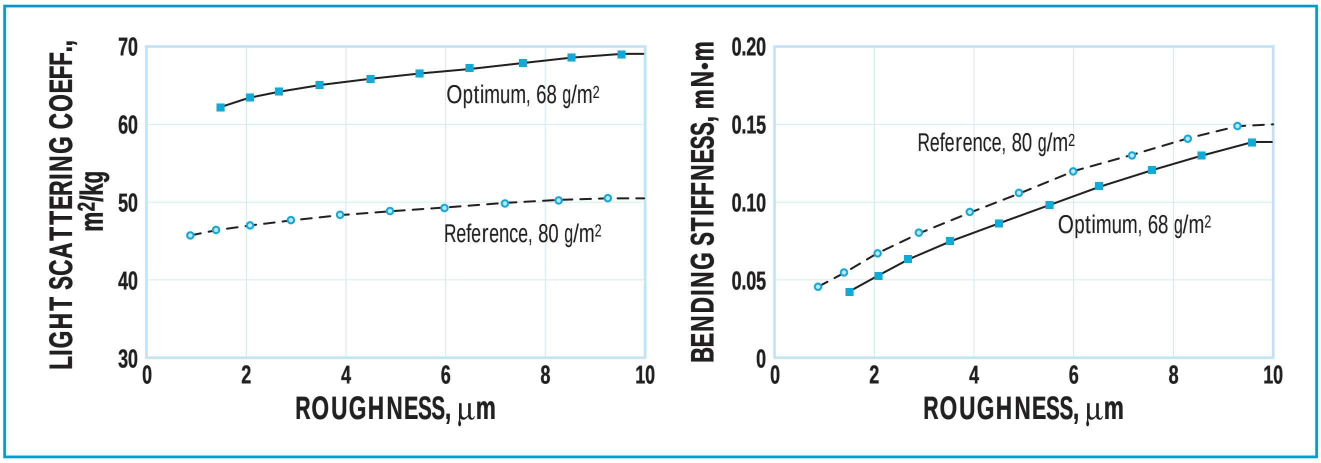
III. Raw material costs in US$/metric ton

CONCLUSIONS

The examples show that structural simulation is an effective approach for comparing paper properties. In the cases studied, one would have had to prepare and measure several thousands of handsheets if the same study were carried out in a laboratory. All the work reported here was done in only eight days.

KCL-PAKKA simulations do not necessarily give the same results as handsheet experiments would give. However, handsheets themselves are not the same as machine-made paper either. In the end, one always needs to test the predictions in actual practice runs. Structural simulations can be used to guide such experiments in the same way as can traditional handsheet studies, but these simulations are much faster.

KCL-PAKKA simulations require information about the fiber properties. If the information is not readily available, such as from previous case studies, it can be obtained by comparing simulation results with the results of a few handsheet trials. The simulations can also be utilized to explore a new combination of pulp properties and to evaluate its potential in papermaking. TJ



3. Light scattering coefficient and bending stiffness versus roughness in the simulated copy paper calendered by the model.

	Mass fraction, %	Length, mm	Coarseness, mg/m	Wet flexibility, 10^9/N·m²
Old newspaper				
Long	30	2.2	0.352	10
Medium	20	1.7	0.224	20
Short	20	1.2	0.080	30
Fines	30	0.03	n/a	infinite
Pine kraft				
Long	30	3.4	0.350	40
Medium	40	2.1	0.198	50
Short	20	1.0	0.082	80
Fines	10	0.03	n/a	infinite
Birch kraft				
Long	10	1.8	0.202	200
Medium	40	1.0	0.149	300
Short	40	0.7	0.096	400
Fines	10	0.03	n/a	infinite

IV. Properties of fiber fractions in the folding boxboard case

	Reference	Optimum
Grammage, g/m²	45 + 190 + 45	39 + 202 + 39
Pine kraft in top plies, %	20	60
Filler in top plies, %	5	8
Density, kg/m³	537	518
Bulk, cm³/g	1.86	1.93
Y-value, %	78	76
Bending stiffness, mN·m	30	29
Tear strength, mN	2021	2050

V. Properties for the reference and optimum in the folding boxboard case

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LITERATURE CITED

1. Niskanen, K. J. and Alava, M. J., *Phys. Rev. Lett.* 3(25): 3475(1994).
2. Nilsen, N. and Niskanen, K., *Progress in Paper Physics—a Seminar*, STFI, Stockholm, 1996, p. 19.
3. Görres, J., Amiri, R., Wood, J. R., and Karnis, A., *Tappi J.* 79(1): 179(1996).
4. Steadman, R. and Luner, P., "The Effect of Wet Fiber Flexibility on Sheet Apparent Density," in *Papermaking Raw Materials* (V. Punton, Ed.), Mechanical Engineering Publ., London, 1985, pp. 311–338.