Simulating Colloidal Thickening: Virtual Papermaking

J. Scharcanski † and C.T.J. Dodson ‡
† Institute of Informatics
Federal University of Rio Grande do Sul, Porto Alegre, Brasil 91509-900
and
‡ Department of Mathematics
UMIST, Manchester, U.K. M60 1QD

October 1, 1999

Abstract

Paper is made by the continous thickening of an aqueous suspension of cellulosic particles. In published computer simulations, the interactions among cellulose fibers have mainly been considered the most relevant issue. However, colloidal particles are present in much larger numbers than cellulose fibers, and influence paper quality in different ways. In this study, we describe a new simulation procedure for the interactions among fibers and fines, during the thickening process. Among the parameters involved in paper forming taken into consideration are fiber and fine size distributions, fiber and fine concentration, fiber propensity to flocculate, fiber flexibility, as well as parameters describing the process conditions, like geometry of the filtering fabric, drainage speed, turbulence intensity and turbulence decay. Generated structures may be useful in interpreting physical processes in the forming process, design of new measuring instruments or estimation of product quality.

Keywords SIMULATION, FORMING, STRUCTURE, FIBERS, FINES

1 Introduction

Papermaking is a complex process because of its nonlinear and stochastic nature. An aqueous suspension of cellulosic fibers, fiber debris and some filler solid particles like clay or chalk is drained in a continuous process involving one-sided or two-sided dewatering at high speed. Typical natural cellulose fibers are of rectangular cross section, a millimeter or two long, 30 micrometers in width and about 5 micrometers thick; fiber debris, called 'fines' consists of broken particles of fiber with characteristic dimension less than about 200 micrometers. The rather high aspect ratio and flexibility of cellulose fibers result in a high propensity to aggregate or 'flocculate' through mechanical entanglement, giving rise to clumps or 'flocs'. Filler particles have typical dimensions of a few micrometers and impart or enhance specific sheet properties, or to serve other necessary purposes [1]. Such additives as alum, sizing agents, mineral fillers and others are commonly used for purposes that include: pH control (acidity), control of penetration of liquids, or the improvement of optical and surface properties.

Paper quality and paper machine operation are affected by properties of fibers and non-fibrous additives. Some of the major factors that affect the forming process are suspension concentration, fiber and fabric characteristics, machine speed, types and amounts of additives (e.g. fillers, mineral particles, and others). The complex interactions among constituent particles and the chemical and/or physical processes during paper forming, develop at the mechanical, colloidal and molecular levels. There is a wide range of phenomena that influence these fundamental interactions. Some important physical and chemical factors in these phenomena are surface charge, fiber entanglement, flocculation, coagulation, hydrolysis, and time-dependent chemical reactions [1]. Quantitative modeling of such complex chemical and physical processes still lacks the fundamental understanding of the physics of the overall papermaking process.

Therefore, many decisions about forming issues (e.g. parameter setting) are empirical, instead of being based on objective criteria. This leads to sub-optimal system operation, and ultimately, less profitability. Recently, simulations have been used to provide insight on the processes of fiber aggregation (i.e. flocculation) and disaggregation (i.e. dispersion), as well as on the evolution of the web on paper formers [2] [3]. These simulations tend to emphasize the dynamics of cellulose fiber networks. However, additives such

as colloidal particles (i.e. fines) constitute a relevant percentage of the total sheet mass (usually, between 10-30%), and exist in overwhelming numbers compared to fibers. Also, fines influence paper forming and several paper properties, such as porosity, floc size, and floc density. However, most simulation procedures reported in the literature do not consider fines. The development of such simulation procedure still is a challenging research issue. It could help us understand better the physics of paper formers, predict the effect of different forming parameters on paper quality more accurately, and, perhaps, augment control procedures.

This study proposes a new simulation method, based on a modified version of the model proposed in [2]. This method simulates paper forming at the mechanical and colloidal levels, in terms of fiber entanglements and their interaction with fines. Due to the large number of fibers and fines interacting during pad consolidation (i.e. paper forming), the computational cost could become prohibitive if objects were to be considered two, or three, dimensional. Therefore, the forming process will be represented in one dimension, so computational complexity can be reduced. This is achieved by projecting a random scanning line onto the plane of the forming web, and observing the locations of the fibers and fines as crossings on the scanning line. The simulation of the dynamics of fiber and fine interactions during paper forming, is based on this set of crossings. Different forming conditions are represented by the state of the different forming parameters. The next sections present details of the proposed approach, with several illustrative results and applications.

2 Modelling the Interaction Among Fibers and Fines

This simulation focuses on the collective behavior of the fiber and fine aggregation and disaggregation taking place in fibrous networks during the forming process, and different parameters are taken into consideration.

Fibers may interact with other fibers and/or fines. The dynamics of such interactions can be described by saying that in low turbulence fibers and fines aggregate into flocs (clumps or clusters), in high turbulence flocs may disintegrate into their component fibers, and this may be iterated. It is a continuous process, taking only a few tenths of a second until a stable condition is achieved during the dewatering and pad consolidation. A two-dimensional illustration of simulated fibers and fines interactions during paper forming may be found in Figure 1. In this example, we used just 70 fibers and 30 fine elements. In the initial state, fibers and fines are randomnly positioned, as Figure 1(a) shows. After a short time (i.e. a few simulation steps), fiber clumping and the tendency of fines to stick to fibers are already noticeable (please, see Figure 1(b)).

Several process parameters are considered in this simulation procedure. For example, fiber and fine tendency to disperse in the fluid medium, the decaying turbulence on the forming fabric, and the tendency of fibers in the suspension to concentrate around drainage vortices (fabric pores) when fluid is being drained from the suspension). In this study, we focus on the effect of aggregation of fibers and fines.

The simulation starts from a random distribution of fibers and fines; this is a realisation of a composition of Poisson processes on the scanning line, so intercrossing distances are exponentially distributed. This initial state of the simulation represents the fiber and fine crossings y_i distribution on a random scanning line, assuming that fibers and fines are not flocculated (i.e. not clumped) at this stage of the forming process. Fiber and fines interact only if they are located within a certain distance of each other, because fines may be seen as colloidal particles in a suspension [5], and, at a close range are attracted to fibers and/or other fine particles. However, if positioned beyond this range, fines are repelled, or the strength of their interaction with other elements in the suspension may be neglected. Therefore, it may be assumed that fiber and fine interactions occur only if they are located within *interaction ranges*, which are proportional to their effective sizes (i.e. *fiber length* and *radii of fine particles*). It is known that *fiber length* can be modelled by the *lognormal distribution*, as also can particles generated by fractioning (such as fines) [4]. These *fiber lengths* and *fine radii*, which are generically denoted by y_i^r, are used to estimate the local *interaction ranges*.

Different simulation parameters correspond to distinct operating conditions of a *virtual paper machine*, and distinct paper structures. The proposed model is simply a linear combination of effects of the individual components mentioned previously. This is described by the following difference equation [2]:

$$y_i^{'} = y_i + G(t)(\Delta y_i) \tag{1}$$

where the y_i are the coordinates of fiber crossings on a random scanning line, and $G(t)$ expresses a decay in the fiber network activity as the dewatering process develops. Eventually the network converges to a stable state as the simulation time $t \to \infty$. This activity decay results from the decrease in the amount of fluid, and consequent reduction of the fiber mobility in the fiber network. This decay has been modelled as a *negative exponential* because of the *filtration effect*, which implies that the resistance to fluid drainage increases as more mass is deposited on the forming fabric (in the vicinity of the drainage points), and is inversely proportional to the pressure differential across the fabric.

The term (Δy_i) (in Equation 1) is the summation of linear motions imposed on a fiber crossing y_i, by the factors mentioned previously :

$$(\Delta y_i)^{'} = (\Delta y_i)_{flocc} + (\Delta y_i)_{disp} + (\Delta y_i)_{turb} + (\Delta y_i)_{drain} \tag{2}$$

where, $(\Delta y_i)_{flocc}$ is the effect of the *fiber propensity to flocculate*, $(\Delta y_i)_{disp}$ is the effect of *propensity of fibers to disperse*, $(\Delta y_i)_{turb}$ is the *turbulence* effect, and $(\Delta y_i)_{drain}$ is associated with the *smoothing due to preferential drainage* effect. The modelling and derivations of these parameters, as well as difference equations convergence in the limit, are extensively discussed in [7]. However, the introduction of fines in the flocculation/aggregation process is discussed next.

The aggregation of fibers and fines process during paper forming, is described by the following difference equation :

$$(\Delta y_i)_{flocc} = \begin{cases} \alpha(y_{i+1} - y_i) & \text{if } (y_{i+1} - y_i) \leq (y_i - y_{i-1}) \text{ and } (y_{i+1} - y_i) > (y^r_{i+1} + y^r_i) \\ \alpha(y_{i-1} - y_i) & \text{if } (y_i - y_{i-1}) < (y_{i+1} - y_i) \text{ and } (y_i - y_{i-1}) > (y^r_i + y^r_{i-1}) \end{cases} \tag{3}$$

where α is a constant associated with the *propensity* of fibers and fines to aggregate, y_j are crossings with the scanning line, and y^r_j are the *effective radii* of interaction for each crossing.

Our simulation has two steps, namely: fiber-fine mixture specification, and fiber-fine dynamical interaction. It has been reported that in so-called 'mechanical' fiber pulps made by grinding wood chips, fines are retained within the fiber network only up to a percentage of the fibrous density (in g/cm^3) [6]. Higher densities do not change the structure. Therefore, to be consistent, our model *saturates* when the *free fiber length* decreases to a minimum, such that further structural accommodation is no longer possible. This condition is better described by an analogy. Let us assume for a moment that fines *stick* to fibers, making fiber width larger. Then, as fine content is increased, fibers get *thicker*. This process develops to a point that virtually no free fiber length is left within the structure. At this stage, any increases of fine content, or further fiber/fine aggregation, will have little effect on the structure. Under these circumstances :

$$(\Delta y_i) = 0 \text{ if } \begin{cases} (y_{i+1} - y_i) \leq (y_i - y_{i-1}) \text{ and } (y_{i+1} - y_i) < (y^r_{i+1} + y^r_i) \\ (y_i - y_{i-1}) < (y_{i+1} - y_i) \text{ and } (y_i - y_{i-1}) < (y^r_i + y^r_{i-1}) \end{cases} \tag{4}$$

Once the simulation reaches steady state, a stable network is obtained, and paper structural properties are defined. Experimental results show that usually this process takes no longer than $\frac{1}{10}s$ in a commercial *paper former* [4]. At this stage, the structural properties should be described using an objective criteria. This is the subject of the next section.

3 Paper Quality and Flocculation

There are several approaches for paper structural description, and for quality evaluation. One of the most important is the degree of fiber clumping, or *flocculation*. It reflects how *uneven* is the mass distributed in the paper sheet. This aspect of the paper structure can be represented by different features. In this work, we focus on the paper *floc* and *porous* structure.

The *floc* structure can be represented by the following features: *mean floc grammage* $\overline{G}$ and *mean floc diameter* $\overline{D}$. Dodson [8] showed that the distribution of flocs can be described by a lognormal density, and its standard deviation σ_D is related to the *mean floc diameter* $\overline{D}$ by:

$$\sigma_D = \sqrt{e^{\sigma^2} - 1}\overline{D} \tag{5}$$

where σ^2 is the variance of the *logarithm of floc diameters* (i.e. $logD$). It is then concluded that :

$$e^{\sigma^2} = \frac{\overline{D}}{e^{\overline{logD}}} \tag{6}$$

Also, Farnood's [10] experimental work showed that for most papers :

$$\sigma_D \simeq 1.2\overline{D}^{\frac{2}{3}} \tag{7}$$

and that $\overline{G}$ and $\overline{D}$ are linearly related, i.e.

$$\overline{G} \simeq 0.28\overline{D} - 0.12 \tag{8}$$

Therefore, we may conclude from the discussion above that if the *mean floc diameter* $\overline{D}$ is known, the floc distribution, which is described in terms of G and D, is also known for practical purposes.

As mentioned before, fiber clumping of *flocculation* can also be characterized in terms of its complement: the paper porous structure. These features lead to *optimal discrimination* of different classes of structures, as will be reported elsewhere. However, in practice it is difficult to measure directly the pore size distribution. Therefore, indirect measurements are of practical interest.

Recently, it was shown that the gamma density represents the fiber inter-crossing distances in flocculated networks, and this function also describes a family of pore size distributions indexed by the degree of flocculation in the network [9]. The gamma distribution has a probability density function given by :

$$f(g) = \frac{b^k}{\Gamma(k)} g^{k-1} e^{-bg} \tag{9}$$

and a particular distribution of fiber inter-crossing distances (i.e. gaps g) is described by the parameters k and b of the gamma. It was verified experimentally that, for commercial samples, the parameters k and b increase with flocculation, and decrease with the areal density of the sample [9]. In fact, these parameters were found to be linearly related, and if k (or b) is known, then b (or k) is also known. Therefore, the parameters k and b,G and D are correlated. In fact, k and b have a physical interpretation. The parameter b is a scale parameter for the mean of the gamma distribution of inter-crossing distances; on the other hand, k represents the positional correlation within the ensemble among fibers and fines: $k = 1$ if fibers and fines are positioned randomly with respect to each other, so there is no correlation; $k < 1$ represents clumping (for surface physical or chemical reasons, depending on the actual suspension constitution); $k > 1$ represents the opposite of clumping, which is tendency to repel one another, again for surface physical or chemical reasons depending on the actual suspension constitution.

However, if we normalize the distribution to have unit mean for gaps, $\overline{g} = \frac{k}{b} = 1$. Then, with $z = \frac{g}{\overline{g}} = \frac{gb}{k}$

$$f(z) = \frac{z^{k_{norm}-1}}{\Gamma(k_{norm})} k_{norm}^{k_{norm}} e^{-k_{norm} z} \text{ for } z > 0,\ k_{norm} > 0. \tag{10}$$

So, equation(10) describes a gamma distribution with variance $\frac{1}{k_{norm}}$ and mean $\overline{g} = \frac{k}{b} = 1$. In fact, the gamma distribution provides a family of models for gap distributions with unit mean gap length and variance $\frac{1}{k_{norm}}$. For $k_{norm} = 1$, a *negative exponential* is obtained, and the represented structure is random. If $k_{norm} > 1$ the represented structure is flocculated, and if $k_{norm} < 1$ the represented structure is dispersed. As will be discussed later, k_{norm} depends only on the degree of flocculation of a particular fibrous network, and does not depend on its areal density or fiber properties.

The properties of the simulated paper will be described using the above features. In order to illustrate the effectiveness of the proposed simulation approach, some results and applications are discussed next.

4 Experimental Results

In general, the information obtained from commercial samples are sparse. Among the reasons for the sparseness of this data are the difficult access to actual parameter settings (i.e. forming conditions), the correlation among parameters, and inaccurate prediction of paper properties based on parameter values. Therefore, simulations complement the data obtained from commercial samples. Within the simulation environment, forming conditions are controllable, the different parameters involved in paper forming can be specified independently, which is very difficult to achieve with real world formers.

In order to verify the simulation performance, one thousand simulated samples were generated, given different forming conditions and fines content. Several features of the resulting fibrous network were computed, and these results are compiled in Figures 2 and 3.

As was observed also in commercial samples [10], Figures 2(a) and (b) show that k and b are linearly related; they decrease with flocculation (so $\frac{1}{k}$ and $\frac{1}{b}$ increase with flocculation). As fines content is increased from 10% to 30%, keeping the other conditions constant, a narrower range of flocculated structures is obtained (i.e. the range of $\frac{1}{k}$ values is decreased). It is noticeable in Figures 2(c) and (d) that as fines content is increased, local areal density variance is decreased, at all levesl of flocculation. This shows that our simulation procedure reproduces correctly the *space filling* and smoothing effect studied by Gorres et al. [6].

A careful analysis of Figures 3(a) and (b) show that variance of local areal density, local gradient magnitudes, and the variance of gap sizes between pairs of adjacent crossings are linearly related. In practice, gap size distributions are measured off-line, but faster measurements are highly desirable. The gap size distribution could be estimated indirectly, calculating the local gradient magnitudes, and using the empirical linear relationship. This suggests that gap (and pore size) distributions can be estimated based on optical measurements. In other words, measurements of local areal density variability and local areal density gradients [11], which are faster and less costly than the available porosimetric techniques, can be used to estimate the gap (and pore) size distribution. Also, Figures 3(c) and (d) show the linear relationship existing between G and D, and the degree of flocculation of a structure, indexed here by $\frac{1}{k_{norm}}$. Therefore, as fines content is increased, floc diameter D is decreased in average, following the trend of local areal density variability (see Figures 2(c) and (d)).

Another application of the simulated data is worth mentioning. Once the network reaches steady-state, the paper structure is defined, and it can be represented by its 1D areal density profile—corresponding to an arbitrary scan line in the network. The analysis of this profile allows us to draw some conclusions regarding surface quality, and how it relates to the content of fines in paper. Figure 4 shows two distinct areal density profiles, with different fines contents, made under the same forming conditions. It is noticeable that increasing fines content (from 10% to 30%) improves the profile uniformity. This is an important issue for improving printing quality, from the perspective of paper science.

Finally, it should be mentioned that our method can be utilized for the simulation of planar fiber processes that arise in several contexts, with different controlling parameters, such as in paper and non-woven fabric manufacture, blood vessels growth, crystal growth, and many others. Not much is known about their dynamics, or how their parameters settings affect the final structure in several aspects (e.g. the spatial distribution of number of fiber crossings, pore body size distribution, and so on). Therefore, from the obtained simulated structures, several properties may be estimated and compared to experimental data. Possible applications include the analysis of the simulated interconnecting pore network and comparison to porous media in general, which will be discussed elsewhere.

5 Conclusions

The simulation procedure described seems to provide sufficient flexibility to model several forming conditions occurring in practice. This allows interpretation of suspension and process changes through qualitative parameter changes, and an improved range of design tools for the engineering of papers.

Also, the potential contributions to paper science are promising. The simulation results appear to confirm the hypothesis that fines tend to *stick* to fibers, acting as a *buffer* to fiber to fiber interaction and entanglement. Consequently, *fiber flocculation* tends to decrease as fines content is increased, i.e. the structure becomes more uniform. Particularly, fines tend to make the pore structure, local areal density variability, as well as floc diameter, more uniform, which would be expected to improve printing behavior.

Future work will concentrate on improvements on the proposed fibers and fines interaction model, and their relationship to forming parameters. Also, developments on instrumentation design and printing quality, arising from this work, will be reported elsewhere.

Acknowledgements

The authors wish to thank CNPq (Brazilian National Research Council) for support during the progress of this work. Also, thanks are due to Dr. Bill Sampson and Dr. Mitsuo Inoue, for valuable discussions that improved our work.

References

[1] G. A. Smook. *Handbook for Pulp and Paper Technologists.* Angus Wilde Publications, Vancouver 1992.

[2] J. Scharcanski and C.T.J. Dodson. *A New Simulator for Paper Forming Using Neural Network Methods.* **APPITA Journal**, Vol. 48, No. 5, pp. 347 - 350, 1995.

[3] K. Niskanen, N. Nilsen, E. Hellen and M. Alava. *KCL-PAKKA: Simulation of the 3D Structure of Paper.* Proceedings of The Fundamentals of Papermaking Materials, Cambridge, September 21-26, 1997.

[4] M. Deng and C.T.J. Dodson. **Paper: An Engineered Stochastic Structure.** TAPPI Press, Atlanta 1994.

[5] Mitsuo Inoue. *Personal Communication at the Pulp and Paper Research Institute of Canada*, December 1996.

[6] J. Gorres, R. Amiri, J.R. Wood and A Karnis. *Mechanical Pulp Fines and Sheet Structure.* **Journal of Pulp and Paper Science**, Vol. 22, No. 12, pp. 491 - 496, 1996.

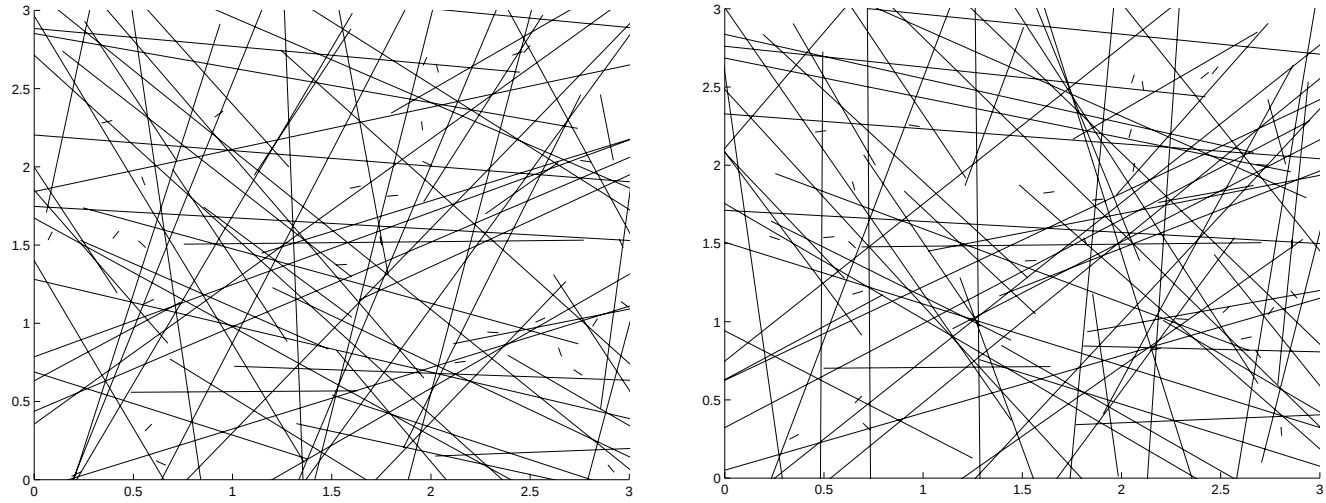
[7] J. Scharcanski and C.T.J. Dodson. *Neural Network Model for Paper Forming Process.* **IEEE Transactions on Industrial Applications**, Vol. 33, No. 3, pp. 826-839, May/June 1997.

[8] C.T.J. Dodson. *Fiber Crowding, Fiber Contacts and Fiber Flocculation.* **TAPPI Journal**, Vol. 79, No. 9, pp. 211-216, 1996.

[9] C.T.J. Dodson and W.W. Sampson. *Modelling a Class of Stochastic Porous Media.* **Applied Mathematics Letters**, Vol. 10, No. 2, pp. 87-89, 1997.

[10] R.R. Farnood. *Sensing and Modelling of Forming and Formation of Paper.* PhD Thesis, Pulp and Paper Centre, University of Toronto, Canada, 1995.

[11] J. Scharcanski and C.T.J. Dodson. *Texture Analysis for Estimating Spatial Variability and Anisotropy in Planar Stochastic Structures.* **Optical Engineering Journal**, Vol. 35, No. 8, pp. 2302-2309, August 1996.



(a) (b)

Figure 1: Fiber and fines interactions : (a) initial state (random spatial positioning); and (b) fiber clumping and fines sticking to fibers after a few simulation steps.

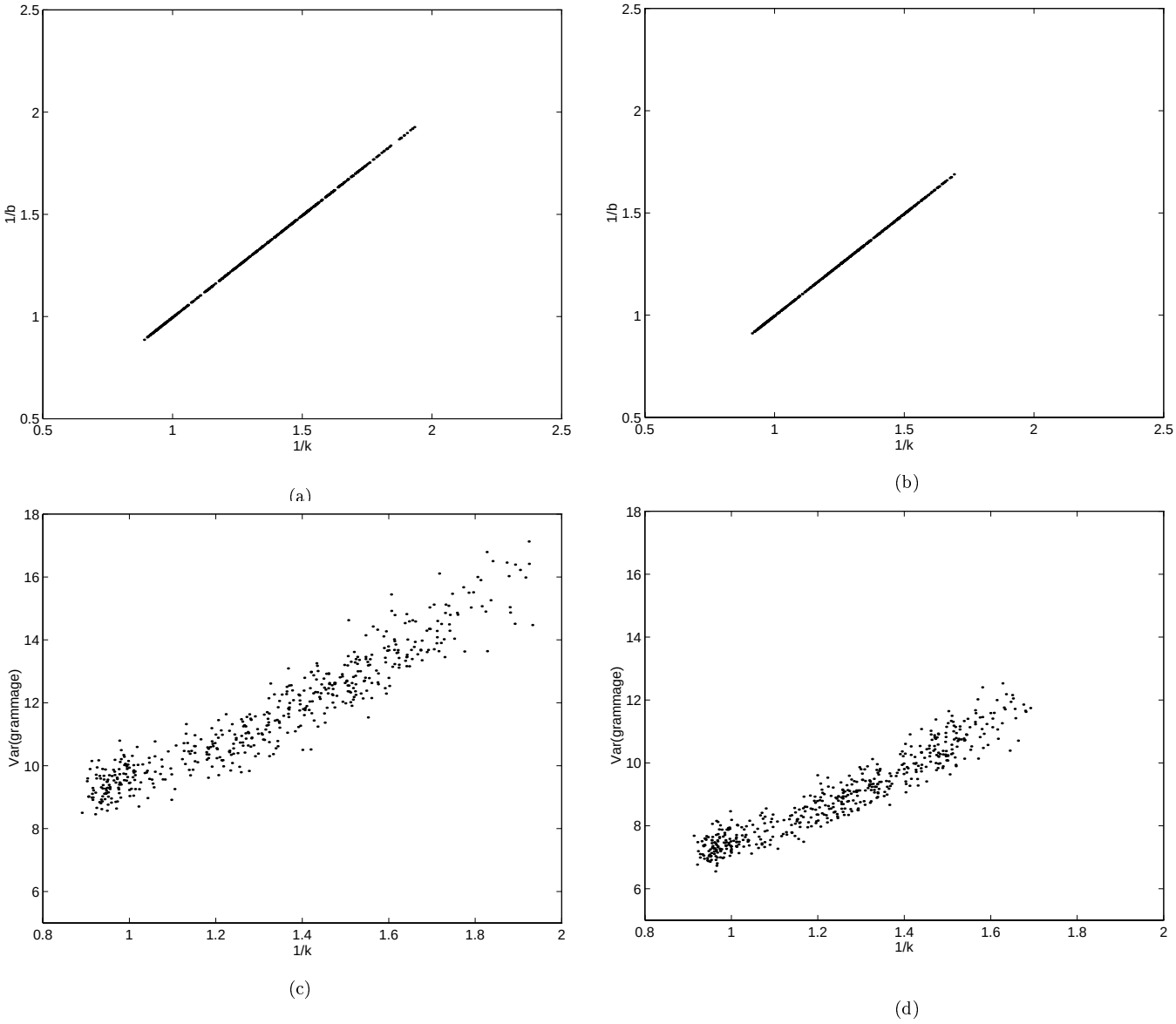
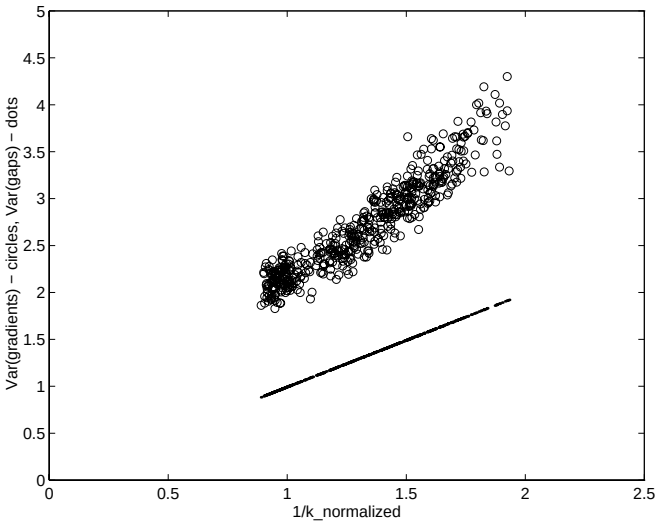
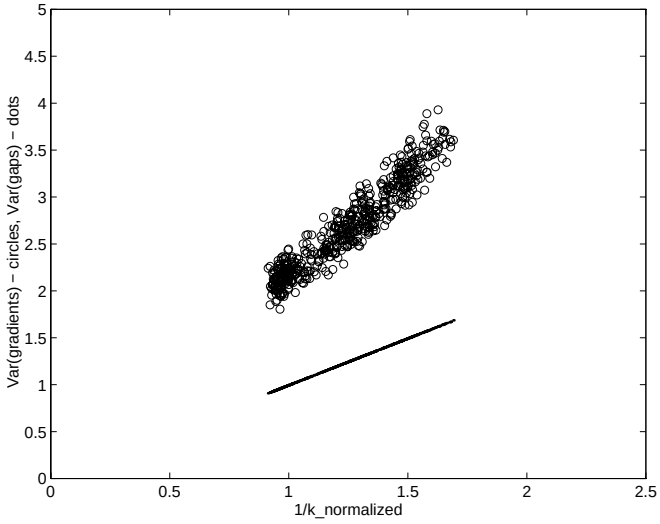


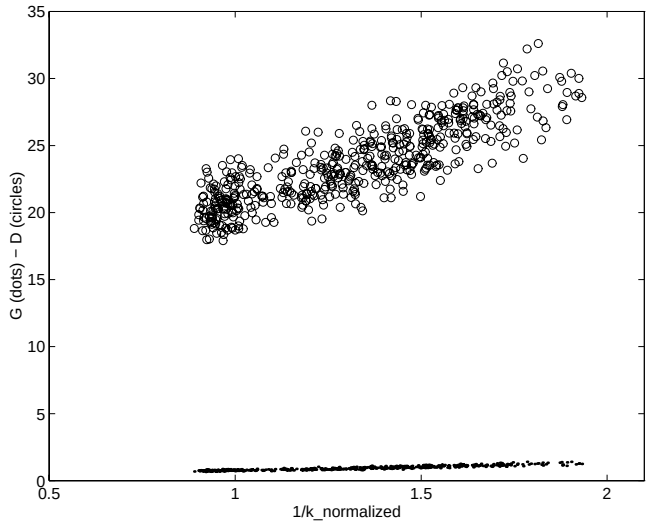
Figure 2: Plots of inter-fiber gap and areal density related features : (a) and (c) 10% fines content; (b) and (d) 30% fines content.



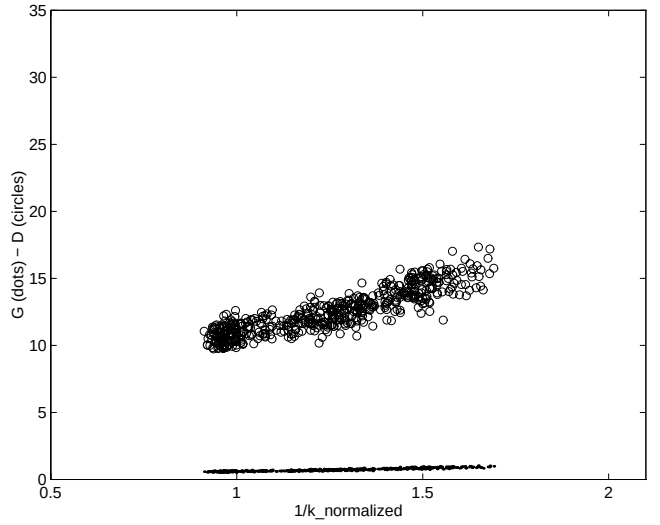
(a)



(b)

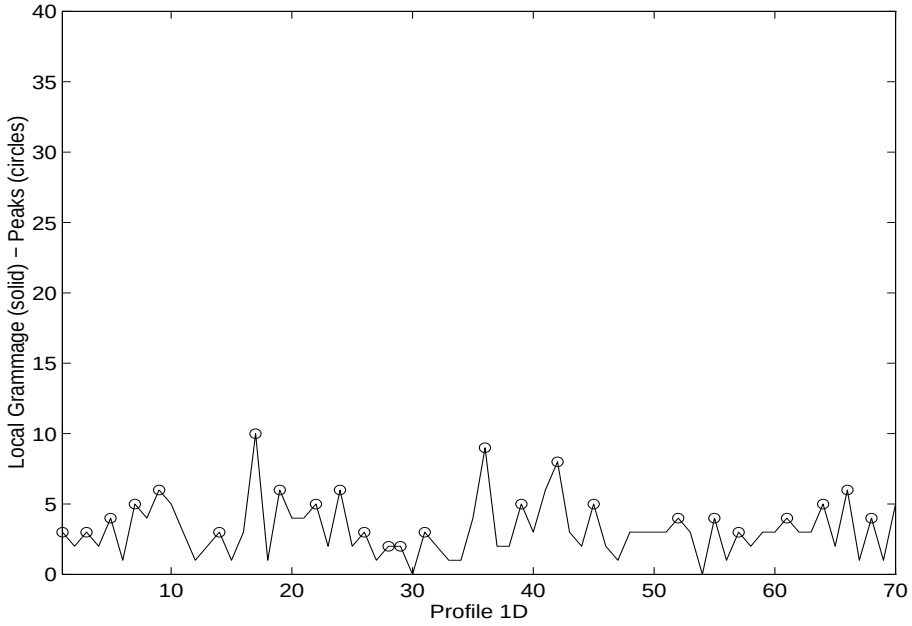


(c)

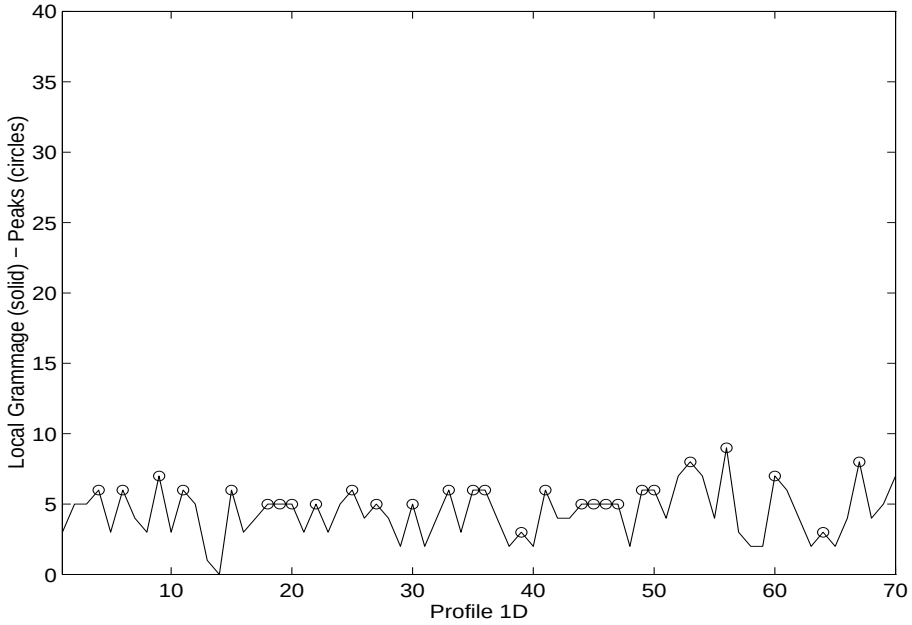


(d)

Figure 3: Plots : Variances of gradient magnitude and inter-fiber gaps versus $\frac{1}{k_{norm}}$ (a) 10% fines content and (b) 30% fines content; G and D versus $\frac{1}{k_{norm}}$: (c) 10% fines content and (d) 30% fines content.



(a)



(b)

Figure 4: Areal density profiles with good structure: (a) 10% fines; (b) 30% fines.