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KERNEL MASS RELATED PROPERTIES OF CEREAL GRAINS

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To Eva, John and Lisa

ABSTRACT

A system for automatic determinations of kernel-mass distributions, and for sorting of cereal grains by mass was developed. The system provides information on the obtained distributions both graphically and through conventional statistical measures.

The relative variation (coefficient of variation) in kernel mass within the examined samples of wheat, rye, triticale, and six-rowed barley varieties ranged from about 20 to 30%.

Distributions of mass enable close analyses to be made of the influence of conditions in the field on kernel growth. This was exemplified in a study of the effects of fungicide use on the average kernel mass, and on the internal variation in mass.

Relationships between size (mass) and other kernel properties are revealed easily on the basis of mass-sorted fractions. Through analyses of kernels within a mass fraction, relationships between, e.g. kernel shape and other properties can be determined. Knowledge about these internal variations is required for optimal sorting, and thereby for optimal use, of grain. The distributions of kernel properties within grain lots are suitable as a basis for studies of variations between stands.

In the thesis, the potential of the ability to sort grain by mass was exemplified in five studies.

1) The relationship between the main dimensions and kernel mass of wheat grains was analyzed at two moisture levels. The dependencies on kernel mass of equivalent dimensions, bulk density and sphericity were studied.

2) The effects of kernel mass and of shape on drying rate of wheat grains were investigated by fitting thin-layer drying curves to semi-empirical and theoretical solutions to the diffusion equation and comparing the derived coefficients.

3) The variations in kernel properties of protein were analyzed in eight wheat varieties. SDS volumes, wet gluten content, and gluten index were used to estimate the value for bread-making of the protein components in the kernels.

4) The relationships between concentration of ergosterol, commonly used as a marker for fungal growth, and kernel mass were analyzed in five winter grain varieties.

5) Extract yields and beta-glucan concentrations were determined for different size barley kernels.

Key words: grain, grains, kernel, mass, weight, size, variation, distribution, property, fungicide, dimension, density, sphericity, drying, thin-layer, protein, ash, SDS, gluten content, gluten index, ergosterol, malt, extract, beta-glucan

LIST OF INCLUDED PAPERS

This thesis is based mainly on the five papers listed below. In the text, they are referred to by their respective Roman numerals.

I. **Regnér, S.** Apparatus for determination of kernel weight distributions in cereal grains and for sorting kernels by weight. Report 166, 1993. Department of Agricultural Engineering, Swedish University of Agricultural Sciences, Uppsala, Sweden.

II. **Regnér, S.** Kernel size and drying rate of wheat grains. Part one. Distributions of physical dimensions and mass. The manuscript was submitted to Journal of Agricultural Engineering Research in December 1994.

III. **Regnér, S.; Nellist, M., E.** Kernel size and drying rate of wheat grains. Part two. Drying rate. The manuscript was submitted to Journal of Agricultural Engineering Research in February 1995.

IV. **Regnér, S.** Content and quality of protein in kernels of wheat. The manuscript was submitted to Cereal Chemistry in February 1995.

V. **Regnér, S.; Schnürer, J.; Jonsson, A.** Ergosterol content in relation to grain kernel weight. Cereal Chemistry 1994, 71 : 55-58.

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CONTENTS

1. INTRODUCTION

This thesis deals with some of the characteristics of cereal grains. The work was focused on distributions of kernel mass, and on relations between mass and other kernel properties within cereal grains lots.

Everywhere in the world, cereal grains are considered as one of the basic foods and feeds (Brooker et al. 1992). In descending order of production (1987-1989), the principle cereals are wheat, rice, maize, barley, sorghum, millet, oats and rye (Kent and Evers 1994). Cereals are grown (1987-1989) on an area corresponding to 5.3% of total land surface of the world. While the area of land used for the production has remained relatively stable, the total yields of wheat, rice and maize have increased significantly over the past 30 years (Kent and Evers 1994). The yearly production (1987-1989) of cereals is about 350 kg per head of the world's population. About half of this amount is used for human consumption, and the other half is used as feed (37%), for process purposes (10%), and as seed (4%). As a source of energy related to land use, rice is the highest yielding crop (38.1 TJ/ha), followed by maize (33.9 TJ/ha) and wheat (27.7 TJ/ha) (Kent and Evers 1994). The highest protein yield is obtained from wheat crops (190 kg/ha), followed by crops of rice (180 kg/ha) and oats (150 kg/ha). Although oilseeds and legume grains are not cereal grains, they are often included among them.

In Sweden, the major cereal crops are wheat, barley and oats (Table 1). There is no production of rice, millet, or sorghum. The maize grown is used for production of silage and corn cob mix. In the period 1991-1993 the average yearly production of cereal grains was about 4.5 10^9 kg (Yearbook of Agricultural Statistics 1994). This corresponds to approximately 530 kg per head of the Swedish population. Production of the bread types of grain (wheat and rye) is about one-third of total. Grain is grown on about 2.9% of the Swedish land surface area.

Table 1
Yearly Production of grain in Sweden (1991-1993)

Grain type	*Production, 10^6 kg*
Winter wheat	1400
Spring wheat	150
Rye	180
Barley	1620
Oats	1180
Oilseeds	290

2. BACKGROUND

Cereals are cultivated types of grass (*Poaceae*). The types of cereals grown to mature crops in Sweden, develop branches only at the base of the main stem. Flowers, and thus seeds, are developed in spikelets. The inflorescences are branched structures. The type of branching varies between species: the spikelets of wheat, barley and rye form ears, while panicles are developed in oats.

Spikelets of wheat can contain up to six florets or more. It is, however, unusual that all florets are fertile. At maturity, central spikelets of wheat ears normally contain three to five kernels, while more distal spikelets (basal and upper) contain only one or two. In the most basal spikelets usually none of the florets is fertile. The number of kernels that develop within the spikelets is partly genetically controlled and therefore varies among varieties (Svensson 1994). Basal florets of central spikelets reach anthesis earlier than upper ones in the same spikelets, and earlier than basal ones in distal spikelets (Rawson and Evans 1970). The differences in developmental stage remain, although reduced with time, throughout the growing season (Kirby 1974; 1977). Differences in final grain weight (Fig. 1) have been attributed more to the rate of dry matter accumulation than to the duration of the grain-filling phase (Housley et al. 1982).

In ears of barley, the spikelets develop in groups of three. Each spikelet contains a single floret. In six-rowed types all spikelets can bear grain, although the centre grain of the three in the group develops better and obtains higher mass. In two-rowed types only the florets in centre spikelets of the three are fertile. As for wheat, kernels in central spikelets of the ear develop earlier, and reach higher masses, than do distal (upper and basal) ones.

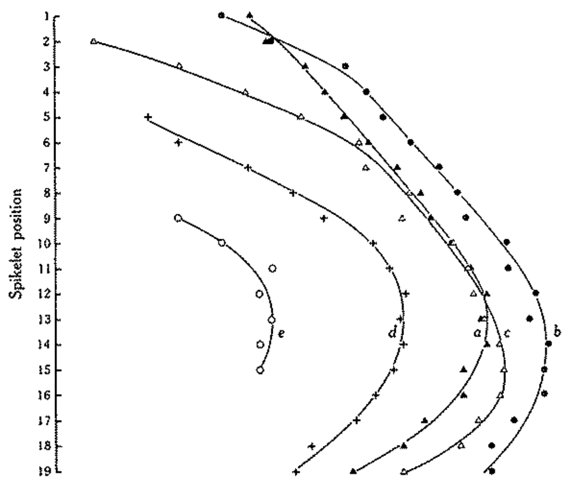

Fig. 1. Typical profiles of grain masses within an ear of wheat. Kernels in the basal florets are designated a and other grains are lettered progressively towards the tip of the spikelet (Bremner and Rawson 1978).

Rye spikelets can contain up to six florets (Kent and Evers 1994), but seldom more than two grains are developed (Geisler 1983). Distal spikelets often contain only a single grain. The kernels developed in central spikelets of the ear are larger than those developed in the distal ones.

In the panicle of oats, the upper spikelets are earlier in development than central and basal ones. Due to the ability of plants of oats to compensate within the panicle, the variation in grain mass between spikelets is lower than the corresponding variations between spikelets in ears of wheat, barley and rye (Geisler 1983). However, within the spikelets the kernels differ in size: the masses of kernels developed in primary florets are about 50% higher than the masses of kernels developed the secondary ones (Geisler 1983). More than two kernels can, but seldom do, develop within spikelets of oats.

Cereal plants are always prepared to develop more kernels in the inflorescences than the number actually produced. The number of kernels that will develop is adjusted in accordance with the conditions during growth. The better the conditions, i.e weather, and accessibility of water and nutrients, the more kernels are developed. The reduction in the number of kernels that will develop proceeds until around the time of fertilization (Åfors et al. 1988). The strategy to reduce the number of kernels when conditions are unfavourable is a result of the plant's desire to produce as many seeds of good quality as it possibly can.

Another possibility for the plant to adjust the number of kernels that develop, and thereby the yield, is to control the number of tillers developed (Åfors et al. 1988). The ability to develop tillers differs between species and varieties (Geisler 1983). The accessibility of water, light, and nutrients also influences the number of tillers developed. If the accessibility of these components is low during the growing period, additional tillers will not develop. If accessibility is severely reduced, the development of the tillers of highest order will cease (Masle 1985). Tillers can develop as late as in the kernel filling period. After rain in sparsely covering crops, late-developed tillers often are present as green unripe ears in the otherwise relatively mature crops.

The flowers of tiller ears reach anthesis later than corresponding flowers on the main shoot ear. The later the tiller is developed the fewer and smaller the kernels will usually be at maturity. The largest kernels within a crop are found in the basal florets of the central spikelets on the main shoot ear of plants with many tillers (Dahlstedt 1985; 1991).

A result of the adjustment of the number of kernels that develop within the ears, as well as the number of tillers that develop on the plants, is that the average mass of the kernels is relatively stable, although the yield may vary significantly.

Normal average masses of kernels of the different types of grain are well known and can be found in the basic literature in agriculture. In many cases it is also known how the average kernel weight is affected by different treatments in the field. Less is known about the variation in mass among the kernels in grain lots, and how the distribution of mass is affected by different treatments. Little is known also about the relationships between the mass and other properties of kernels.

3. OBJECTIVES

The primary objective of the research was to develop a system that enabled us to determine distributions of kernel mass within grain lots, and to automatically sort grain kernels by mass (Paper I). The second overall objective was to use the system to gain knowledge about the mass-related distributions of some important characteristics of grain kernels (Papers II, III, IV, and V).

4. APPARATUS FOR DETERMINING MASS DISTRIBUTIONS, AND FOR SORTING KERNELS BY MASS

The idea to develop an apparatus that could automatically determine the distribution of mass of grain kernels emerged after some time-consuming manual determinations of these distributions. In these manual analyses we found that the masses of the kernels varied significantly within normal samples of grain, and, thus, that large numbers of kernels have to be weighed in order to obtain sufficient data for reliable comparisons between samples.

The system developed (Fig. 2) is described in Paper I. The requirements on the system developed were:

- the kernels should be weighed with an accuracy corresponding to about one percent of their average mass
- all kernels in a sample should be weighed
- the system should be used on a 24-hour basis
- the apparatus should allow simultaneous sorting into at least seven classes
- major components should be purchased, if available
- the system should provide statistical information on the measured kernels for comparisons between samples.

The objective of the development was to obtain a reliable system for scientific studies. Thus, the capacity of the system was not considered as important as would have been the case for a commercial system. The system developed fulfils the requirements set. It has a capacity of about 500 kernels per hour, and enables simultaneous sorting into ten fractions.

An apparatus similar to the one described in Paper I does not seem to have been developed elsewhere. Although some systems described in the literature can, or possibly could, be used to determine mass distributions, none of them was capable of sorting of kernels.

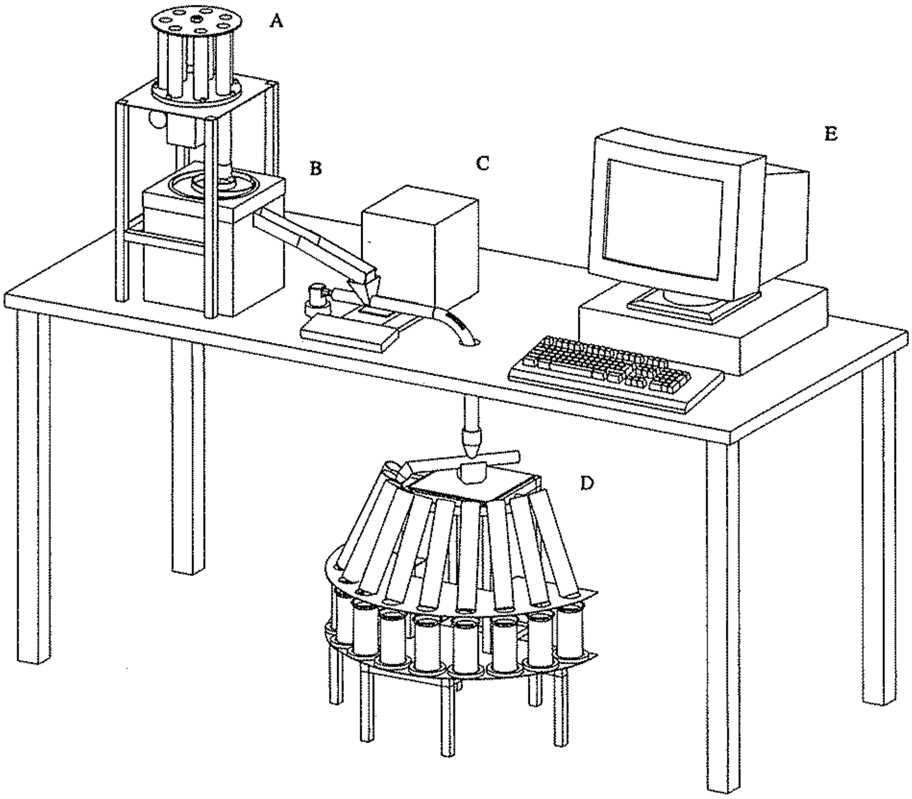

Fig. 2. The apparatus developed consists of five major parts. The sample feeder (A), the kernel feeder (B), the balance (C), the sorting device (D) and a PC (E).

A system constructed primarily for measuring mass, and main dimensions of individual rice kernels was described by Paige et al. (1991). Kernel dimensions were determined by image analysis, and the weighing system was based on a modified 1-mA d'Arsonval meter movement. The capacity of the system was about 30 kernels per minute. Repeated measurements (20 times) on 15 rice kernels showed that the accuracy and repeatability of the system was satisfactory. The authors concluded that after modifications there should be no impediment to a similar apparatus being developed to measure other types of kernels.

In another apparatus, developed for determinations of kernel hardness, kernels were crushed at a rate of about 180 kernels per minute (Martin et al. 1993). Due to the decreasing gap between the rotor and cresent in the apparatus, the time required for crushing a large kernel was longer than that for crushing a small one. A test performed with sifted samples showed that the time required for crushing was not solely dependent on the size of the kernel; the hardness of the kernels also influenced the time required. Because kernel hardness is a genetically determined trait (Hoseney 1987), the hardness should not vary significantly between kernels in a sample of a single variety. Hence, the apparatus could possibly be used to estimate distributions of kernel mass. The results obtained must, however, be corrected in accordance with the varietal kernel hardness.

GrainCheck 310 (Agrovision AB, Lund, Sweden) is a commercial instrument for collecting and analysing video images of grain. Agrovision AB stresses that the instrument identifies different types of grain, damaged or green kernels as well as non-grain material. In addition, the instrument should be able to estimate bulk density, thousand kernel weight, and size distribution (length, width and area). The system is based on two-dimensional measurements and analyses are performed on 50-100 g samples. Neural network is used in the analyses of the video images. Based on the size distributions, the system could probably provide estimates for variations in kernel masses within grain samples.

The accessibility of soft-ware for image analyses, and for improved analysis of data, together with the increased capacities of computers, has enhanced the possibilities for image analysis of grains. New instruments, and new possibilities based on this technique will probably be introduced on the market in the near future.

5. DISTRIBUTIONS OF KERNEL MASS IN GRAIN LOTS

Although it is a well-known fact that masses of grain kernels vary, no information was found in the literature dealing with normal levels of variation for the different types of grain.

As part of the studies concerning the development of stands of spring and winter wheat, Dahlstedt (1985; 1991) manually weighed kernels representing different parts of the stands. In typical mature stands of spring wheat, the kernel masses ranged from 1 to 70 mg. Most distributions representing total stands were skewed towards the kernels of high masses. When specific parts of the stands were selected, for example the main shoot ears of plants, lower levels of variation were obtained, but generally the negative skewness of the distributions remained. Degree of tillering was inversely correlated with the variation in kernel mass. Dahlstedt (1985; 1991) did not present the level of any statistical measure describing the variation in kernel mass. However, a typical distribution (Dahlstedt 1991) of mass in a stand of spring wheat was plotted (Fig. 3). Because the ears were manually threshed, the grain sample contained more kernels of low masses than it would if the crop had been combine-harvested.

Grieve et al. (1992) studied the effects of soil salinity on the yield of main ears. The manually harvested (main) ears were analyzed closely; the numbers of spikelets per ear, and kernels per spikelet were counted. The mass of each individual kernel was also determined. Lesch et al. (1992) used the data gathered to statistically model the configuration of kernels in main ears of salt-stressed wheat.

Regnér (*unpublished*) determined the distributions of kernel mass for 72 samples of spring wheat (four varieties, three locations, three N-levels, and with and without fungicide treatment), and for 63 samples of winter wheat (seven varieties, three locations, and three N-levels). The samples were obtained from field trial plots harvested in 1989. Values of the statistical measures used to describe the distributions obtained are presented in Table 2. Skewness was calculated in accordance with the method used in SAS (SAS 1989). For kernel masses distributed normally the skewness is nil, whereas negative values were obtained for distributions skewed towards the larger kernels. The higher the positive skewness, and the lower the negative skewness, the more skewed were the distributions. Each sample consisted of about 1000 kernels. Samples were only slightly cleaned before the analysis. Although the average mass differed between the kernels of spring and winter varieties, the average relative variations (coefficient of variation) in kernel mass were about the same for the samples of spring and winter varieties (Table 2). The distributions of mass were generally skewed negatively. In an analysis of the values obtained for the statistical measures, variety and location were each found to have a statistically significant influence on the standard deviations of kernel masses, and on the coefficients of variation ($P<0.001$). While both variety and location influenced the skewness of the samples of winter varieties ($P<0.001$), the influence of variety on the skewness of the samples of spring varieties was not significant ($P>0.05$). The influence of rate of nitrogen applied to plots on the variation in kernel mass was less significant than the influences of variety and location. Skewness was negatively influenced by the rate of nitrogen applied, i.e the distributions tended to become more skewed towards the larger kernels the higher the rate of nitrogen applied.

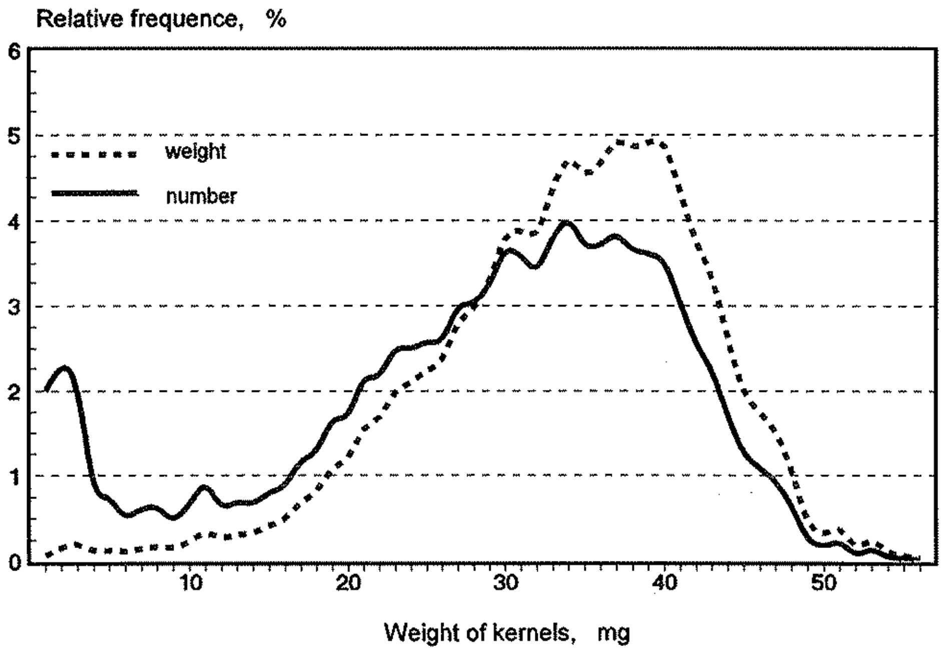

Fig. 3. Typical distribution of kernel mass in spring wheat (Dahlstedt 1991).

Table 2
Average values, standard deviations, and ranges of measures characterizing the distributions of kernel mass in samples of spring (n=72) and winter (n=63) wheat

	Average mass, mg		*Std deviation, mg*		*Coefficient of variation, %*		*Skewness*	
	spring	*winter*	*spring*	*winter*	*spring*	*winter*	*spring*	*winter*
average	37.3	41.6	8.9	10.1	24	24	-0.55	-0.66
std.dev.	1.2	3.4	0.7	1.1	2	2	0.18	0.32
minimum	34.6	32.5	7.2	8.0	19	20	-0.96	-1.20
maximum	40.1	47.0	10.4	13.1	28	29	-0.04	0.02

Five samples of different varieties of barley (three two-rowed, and two six-rowed) were, in 1992, analyzed for their internal distributions of kernel mass (Regnér, *unpublished*). The average masses were lower for the six-rowed than for the two-rowed varieties. The variations in kernel mass, however, were higher for the six-rowed than for the two-rowed varieties. The values of the coefficient of variation (CV) were 20% for both six-rowed varieties, and 13, 14, and 18% for the two-rowed varieties. The grain in the original lots had been cleaned before the samples were taken (aspiration, and screening: oblong holes, width 2.5 mm). Despite the cleaning, the values of the CV for the six-rowed varieties were in the range of those presented for samples of wheat (Table 2). For the two-rowed varieties lower values of the CV were obtained. The different levels of the CV for the two types of barley were probably caused by the different configurations of kernels within ears.

Only one sample each of rye and triticale were subjected to analysis of the kernel mass distribution with the apparatus developed (see Paper V). The variations in mass among kernels of these species were within the range of variations obtained for wheat (Table 2).

In 1993, three commercial samples of oats were analyzed for their internal distributions of kernel mass (Regnér, *unpublished*). The appearance of one of the distributions was exceptional (Fig. 4, left); the distribution contained two marked peaks, each with relatively low width. The distributions of the other two varieties resembled each other. One of these distributions is presented in Fig. 4 (right). The relatively wide top of this distribution is probably due to the two peaks in this case coinciding with each other because of a smaller difference between the average kernel masses of the peaks. The presence of two peaks in the distributions for samples of oats is explained by the different size of kernels that developed in primary and secondary florets of the spikelets, and by the ability of oats to compensate within the panicle.

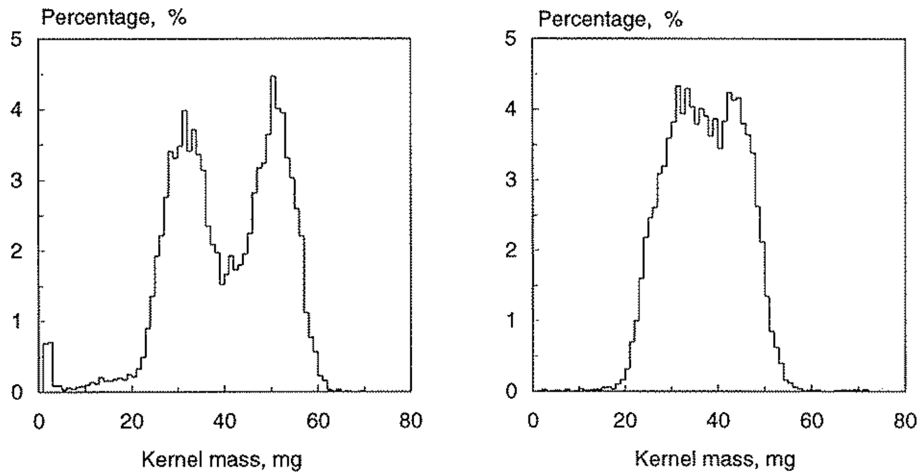

Fig. 4. Distributions of mass within two varieties of oats.

The majority of the grain samples analyzed with the system developed have originated from Swedish crops. A few samples of wheat originating from crops grown in other countries (Canada, and United Kingdom) have also been analyzed. The distributions of kernel mass obtained for these samples were similar to those obtained for Swedish wheat varieties.

6. POSSIBILITIES WITH THE SYSTEM DEVELOPED

That the determination of distributions of kernel mass is made automatically enables the weighing of large numbers of kernels. Because of the high variation in mass among kernels, this is essential for the accuracy of the values of different statistical measures calculated from weighing data. In fact, the magnitude of the variation in kernel mass determines the influence exerted by the number of kernels weighed on the accuracy of the values calculated.

Distributions of kernel mass, and the statistical measures describing them, can better explain the effect of different field treatments on kernel growth than can the average kernel mass, or thousand kernel weight. The closer analysis makes it possible to determine whether an increased average mass was due to an overall increase in kernel mass, or if it was a specific group of kernels whose masses increased. Although the average mass values for two samples may be identical, the variations in kernel mass can differ significantly between them.

Sorting of kernels by mass enables analyses to be made of how other properties of kernels vary with their mass. Because the grain can be sorted into many classes of narrow widths the data obtained is suitable for regression analyses. Together with the distribution of kernel mass, the relationship fitted can be used to model the effects of kernel sorting on the properties of interest.

Using fractions of grain already sorted by mass, the ability of different methods to sort grain for a certain purpose can be studied. This procedure eliminates the influence of kernel mass on the property of interest. Hence, the variation in the specific property among kernels can be determined in several dimensions; the variation with mass, and the variations with the kernel properties on which different sorting methods are based. The optimal way to divide a grain lot can thereby be determined.

Knowledge of the internal variations in kernel properties can serve as a basis for models developed to explain differences in properties between grain lots.

7. SOME STUDIES BASED ON DISTRIBUTIONS OF KERNEL MASS

7.1 Influence of cleaning on the average kernel mass

The average mass of the kernels in a grain sample and the magnitude of most statistical measures describing the variation in kernel mass, normally change if the sample is being cleaned. This is due to the fact that not only non-grain material is removed by the cleaning; kernels of relatively low masses usually separate with the impurities. Thus, the adjustment of the cleaning device also influences the amount of kernels removed. The higher the amount of small kernels removed, the higher the average mass of the remaining kernels will be.

The effect of different degrees of cleaning varies with the purpose for which the grain is to be used. While each kernel has the same importance in germination tests, the influence of individual kernels is dependent on their mass if the sample is to be ground into meal. Thus, even if a kernel property varies significantly with the kernel mass, the amount of small kernels, and hence the average kernel mass, may vary significantly without hardly influencing the content in the meal. In such cases, the median mass of the kernels is a better estimator of the properties of the grain than the average kernel mass. The median mass is the mass that divides a sample into two parts of equal total masses, whereby all the individual masses of the kernels in one of the parts are higher than the median mass, and all masses of the kernels in the other part are lower than the median mass.

The effect of different degrees of cleaning on the average kernel mass and on the median mass can be modelled with the PC-program developed for analyses of weighing data. This is exemplified by an analysis of the distribution of kernel mass in a sample of wheat (SW2 in Paper IV). Considering all kernels with a mass lower than that dividing the distribution as removed, the average and median masses of the remaining kernels were calculated. In Fig. 5 the average and median masses are plotted against the mass of the smallest kernels considered to remain in the sample.

At low levels of cleaning, the rate of increase with the degree of cleaning was higher for average kernel mass than for the median mass. If all kernels with masses lower than 19 mg would be removed, the average mass of the remaining kernels would be 0.5 mg higher than that for the original sample. Meanwhile, the median mass would

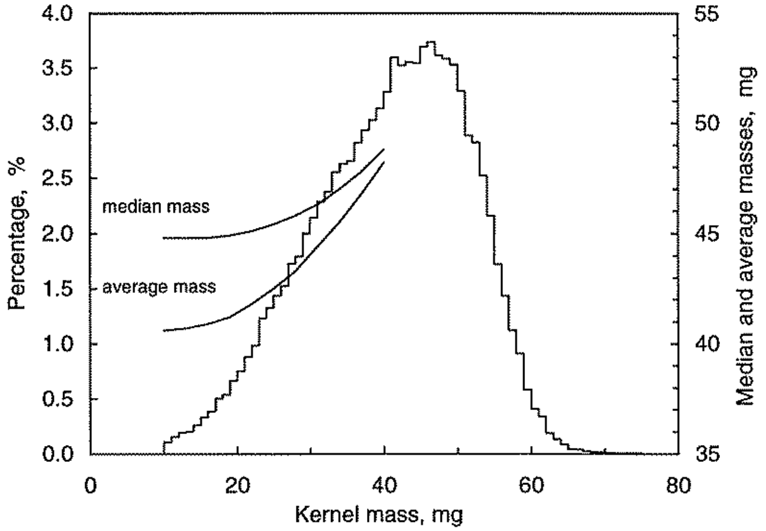

Fig. 5. *Effects of removal of kernels of low mass on the average mass and on the median mass of the remaining kernels.*

hardly change. The removal of these kernels would lower the total mass of the sample by about one percent. Removal of two percent of the sample's total mass, would give an average mass 1.0 mg higher than that of the original sample. The corresponding increase in the median mass would be about 0.3 mg. If five percent of the total mass of the sample was removed, then the mass of the average and median kernel would be 2.2 and 1.0 mg higher than the masses of the corresponding kernels in the original sample, respectively. These calculations have revealed the approximate magnitudes to which different degrees of sorting could influence the average and median masses for a normal grain sample. Higher influence of cleaning would be obtained for samples containing larger relative amounts of small kernels.

7.2 Confidence in average kernel mass - number of kernels measured

The reliability of the average mass estimated for kernels in a grain lot is influenced by the variation in mass among kernels and the number of kernels being analyzed. Assuming that the method used for sampling is irreproachable and the masses of the kernels are distributed normally, Eqn 1 can be used to calculate the limits of a confidence interval for the estimates (Wonnacott and Wonnacott 1972). The calculations require that the standard deviation of kernel masses in the grain lot (σ) and the number of kernels that was analyzed (n) is known. For a two-sided 95% confidence interval the value of the normal variable (Z_{Pr}) is 1.96.

$$\overline{X} - \mu = \pm Z_{Pr} \frac{\sigma}{\sqrt{n}} \qquad (1)$$

Eqn 1 was used to calculate the difference between the confidence limits (95%) and the population average ($\overline{X} - \mu$) at four levels of mass variations. In Fig. 6 the differences between the limits (95%) and true average mass are plotted against the number of kernels weighed in the analysis.

To ensure that the estimated average mass in 95 cases out of 100 does not differ more 0.5 mg from the average of the total population (σ = 10 mg), slightly more than 1500 kernels have to be weighed (Fig. 6). At the same level of variation in kernel mass, the limits of the confidence interval deviate as much as 1.4 mg from the true average if as few as 200 kernels are analyzed.

In accordance with the rules of the International Seed Testing Association (ISTA 1976), 1000 kernels should be weighed in determinations of the thousand kernel weight. For this number of kernels, the limits of the confidence interval (95%) deviates by 0.5 and 0.9 mg from the true average for the standard deviations of 8 and 14 mg, respectively.

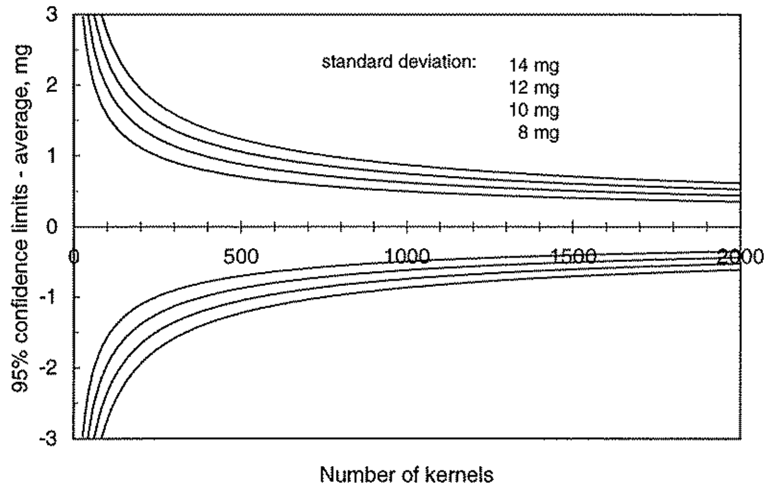

Fig. 6. *Difference between confidence limits (95%) and average kernel mass as function of the number of kernels used in the determination.*

7.3 Influence of fungicides on kernel mass distribution

In a study of the effect of dose of fungicide on yield, a system for linear dose application (Alness 1992) was used. In each of four 20 m long field plots the dose was linearly increased from zero to three times the dose recommended for the fungicide used. The fungicide was sprayed on the crop in late June, shortly before heading. The stands were harvested with a combine-harvester (2.1 m wide) perpendicular to the direction of the dose change. Yields were determined at four levels of application; zero, one, two, and three times the dose recommended. Normally, the increase in yield obtained by the application of fungicides to crops in this developmental stage correlates well with a corresponding increase in average kernel mass.

Samples representing the grain harvested at the four dose levels were each subjected to determination of the internal mass distribution. The average kernel masses were about the same for the corresponding levels of the four plots. The average kernel masses were similar in the samples representing the three highest dose levels. However, the average mass of the grain kernels harvested at the zero level was about ten percent lower. At each level, yields varied more between plots than did the average masses of the kernels. For average values, the relative differences in yield were about the same as the corresponding differences in average kernel mass.

The standard deviations and skewnesses of the distributions were about the same, irrespective of plot and dose. This suggests that the increase in average kernel mass obtained by spraying the fungicide was due to an increase in mass that was of the same absolute magnitude for each individual kernel.

8. MASS-RELATED PROPERTIES OF KERNELS

8.1 Dimensional properties

The size of grain kernels is often described by their main dimensions. The dimensions are moisture dependent; they increase with the moisture content. The average shape of kernels varies between varieties of the same species (Yamazaki and Briggle 1969; Mohsenin 1986). Hence, there is no general relationship between any of the dimensions and the kernel mass. Within a varietal sample, the shape varies between kernels of identical mass. The average shape of kernels also can vary with their masses. No information was found in the literature on relationships between dimensional properties and kernel mass.

8.1.1 *Main dimensions*

In Paper II a study focused on relationships between main dimensions and kernel mass was reported. Main dimensions (Fig. 7) were measured on kernels of two varieties of wheat. Measurements were made at two moisture levels. Before measuring the kernels, they were sorted into weight classes of narrow widths.

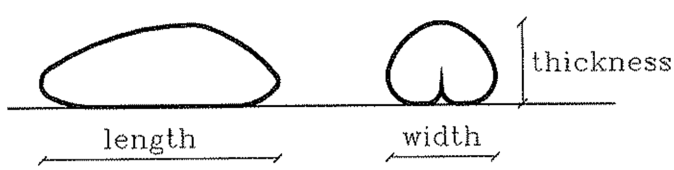

Fig. 7. Main dimensions of a kernel of wheat.

The dependencies on mass of each of the main kernel dimensions were analyzed with a semi-empirical model. The model was based on the relationship between dimensions and mass of identically shaped particles of varying size. For such particles any dimension is proportional to the cubic root of the mass of the particle. This relationship assumes that the density of the particles is independent of their size, which has been found for kernels of wheat (Millet and Pinthus 1984). Because the shape of kernels may be dependent on their size, the physical model was modified to allow for slightly different relationships between the dimensions (d) and mass (m) (Eqn 2). Values of the coefficients a and b were obtained in fits to data on the individual kernels.

$$d = a\, m^{b} \tag{2}$$

For both varieties, the length varied least with mass, and width varied most. However, the dependency on mass of the dimensions varied slightly between varieties. For the Swedish variety Kosack, the values of the dimensionless coefficient (b) expressing the degree of mass dependency were 0.23, 0.35, 0.28 for the length, width, and thickness, respectively. For the British variety Avalon, the corresponding values of the coefficient were 0.15, 0.42, and 0.37, respectively. The larger variation among the values of b for main dimensions of the Avalon kernels, indicates that the shape of the Avalon kernels varied more with mass than did the shape of the Kosack ones. The relationships obtained for the kernels of the Avalon variety are presented graphically in Fig. 8. The averages of the dimensions of the sorted kernels are also indicated.

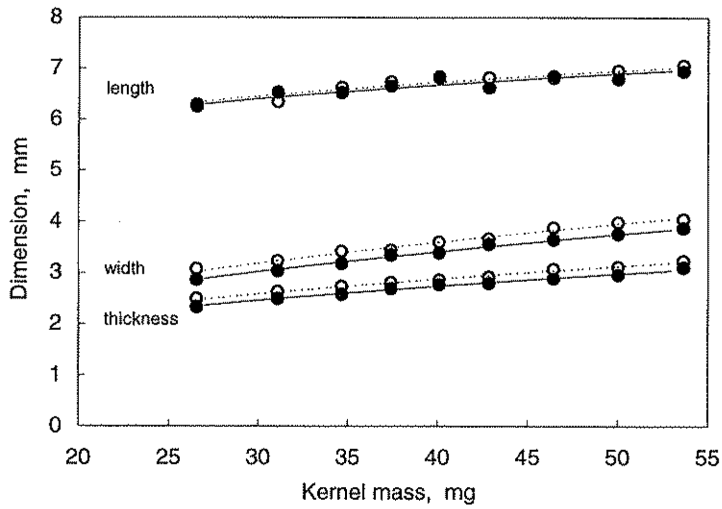

Fig. 8. Average dimensions of the kernels before (unfilled) and after (filled) drying, and curves fitted to data of the individual kernels before (hatched) and after (whole) drying sorted fractions of Avalon.

The dependency on moisture content of each dimension was similar for the two varieties. However, the dependency differed between dimensions; the length varied least with the moisture content, and the width varied most (Fig. 8).

Within weight classes, the variation in each dimension was relatively large. The relationships between length and mass accounted for 33.4 (Avalon) and 53.0 (Kosack) percent of the total variations in length among the kernels measured of each variety. The relationships with mass of width and thickness accounted for between 74.3 and 80.4% of the total variation in these dimensions.

8.1.2 *Equivalent dimensions*

Different types of equivalent dimensions are, instead of the true ones, often used to characterize grain kernels. Equivalent dimensions are the dimensions of regularly shaped bodies, i.e spheres and infinite cylinders and plates, for which the properties should be similar to those of the particle of interest. For wheat kernels, the spherical shape has been proposed to be the most appropriate (Brooker et al. 1992). The magnitude of an equivalent dimension can be calculated by different methods. In the method that is probably most widely used, the dimension of the equivalent particle is calculated from the mass and density of the particle of interest. In Paper II three other methods were used. These are all based on the dimensional properties of the wheat kernels; the geometrical mean, and the surface to volume ratio of spheroids and of rectangular parallelepipeds. Chu and Hustrulid (1968) used the method based on rectangular parallelepipeds for size determinations on maize kernels. Becker (1959) used the one based on the properties of prolate spheroids to relate the sizes of wheat kernels.

The equivalent radii and their dependence on mass varied less between the two varieties than between the methods through which they were obtained (Paper II). The standard deviations of the residuals obtained in the fits of Eqn 2 to data of the individual kernels were in the range 0.03 to 0.05 mm. Because these values were lower than the corresponding ones obtained in the fits of the single dimensions, the equivalent dimensions should provide better estimates of kernel masses than do any of the main dimensions alone.

8.1.3 *Sphericity*

The sphericity, as defined by Mohsenin (1986), is a shape-related measure that is independent of particle size. The sphericity of a sphere is unity, while lower values of sphericity are obtained for other shapes. The sphericity of grain kernels differs between varieties (Mohsenin 1986).

The sphericities of the kernels differed between the two varieties of wheat analyzed (Paper II). Furthermore, the dependency on kernel mass of the sphericity varied between varieties. Whereas sphericities were about the same for all size kernels in one variety (Kosack), they increased with the mass of kernels in the other variety (Avalon).

8.1.4 *Bulk density*

The bulk density of grain is dependent on particle density and the packing efficiency of the kernels. The packing efficiency is dependent on the shape and surface smoothness of kernels (Yamazaki and Briggle 1969). The size of the kernels, however, should not influence the bulk density if kernel size is sufficiently small compared with the volume of grain measured.

Kernels of the same fractions as were used in the dimensional analyses were used to study the dependency on kernel mass of the bulk density (Paper II). The bulk density of the fractions of one variety (Kosack) hardly varied with the mass of the kernels. This was the variety in which the sphericity was independent of kernel size. For the other variety (Avalon), the bulk density of fractions increased with the mass of the kernels. The bulk densities of these fractions were highly correlated to the corresponding sphericities of kernels (Fig. 9).

The bulk densities and sphericities (Fig. 9) obtained for fractions of the two varieties indicate that the packing efficiency varied between varieties and, for one of the varieties, between the fractions of different size kernels. This was supported by the appearance of the kernels. The kernels of the variety (Kosack) with higher bulk density seemed to have smoother surfaces and to be less angular than the kernels of the other variety (Avalon). For kernels of the variety with low and mass dependent bulk density, the angularity seemed to increase as the mass of the kernels was reduced.

The density (particle) of the kernels was not determined. The relatively large difference between the bulk densities obtained for the varieties, and the appearance of the kernels, indicate that most of the varietal difference in bulk density could be attributed to the packing efficiency. However, the somewhat more horny appearance of the kernels of variety Kosack might indicate (Yamazaki and Briggle 1969) that the particle density of the Kosack kernels was slightly higher than that of the Avalon ones.

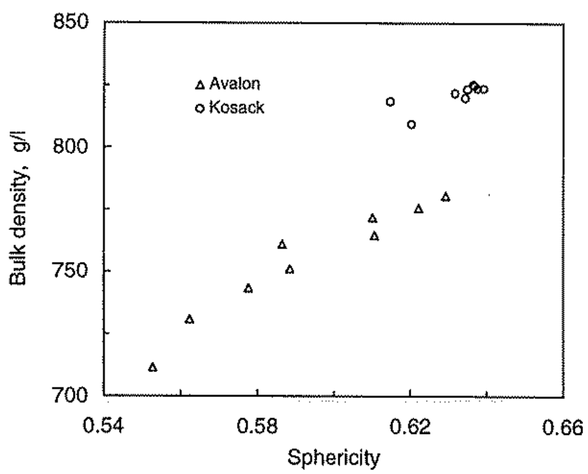

Fig. 9. Bulk densities plotted against average sphericities of the sorted kernels of Avalon (triangles) and Kosack (circles).

8.2 Drying rate

An important characteristic of biological materials is their content of moisture. The concentration of water in cereal grains varies between stages of development. In mature grain, the moisture content is usually too high to allow for immediate storage. If the grain is not preserved, its value might be severely reduced by fungal growth. Drying is the most common method of preserving grain. The accessibility of moisture (water activity) should then be lowered to a level that eliminates fungal growth.

If biological materials are dried for an infinite time they will reach a moisture content that is in equilibrium with the surrounding air. The dimensionless moisture ratio (*MR*) relates the amount of moisture left to be evaporated in the kernels to the amount that totally could be evaporated during the drying process (Eqn 3).

Sometimes, a dynamic equilibrium moisture content (emc) is used instead of the true one. This pseudo emc is often derived in fits of drying curves to drying models, and should be seen as the moisture content the drying product seems to approach using the specific model. However, the final moisture contents in experiments with long exposure times are often lower than most dynamic equilibrium moisture contents presented in the literature.

It is generally agreed that the rate at which water is evaporated from the surface of individual kernels is governed by the moisture diffusion inside the kernels (Brooker et al. 1992; Chu and Hustrulid 1968; Bruce 1985). The drying behaviour of a grain type is normally studied by drying thin layers of a typical sample in high flows of air (Woods and Favier 1993; Bruce and Sykes 1983). The thin-layer drying curves are fitted to theoretical and/or semi-empirical solutions of the diffusion equation, as well as to empirical equations. The Lewis equation (Lewis 1921), the Page equation (Page 1949), the two-term exponential equation (Henderson 1974), and the theoretical solution to the diffusion equation (diffusivity invariate with moisture) (Crank 1956) are examples of models commonly used. All these equations assume constant diffusivity throughout the drying process. Crisp and Woods (1994) used a method that made allowance for time-varying drying temperatures, in fits of drying curves of rapeseed to the theoretical solution for spheres. However, it is generally agreed that the resistance to moisture migration is not solely a function of temperature, it is also dependent upon the moisture content (Brooker 1992; Chu and Hustrulid 1968; Bruce 1985). Then, the diffusion equation has to be solved numerically. Chu and Hustrulid (1968) and Bruce (1985) used finite difference technique to obtain thin-layer drying models for maize and barley, respectively. Bruce (1985) incorporated a time-varying boundary condition for the surface moisture content of the kernels.

Although wheat is one of the most important crops in the world, there is a lack of models capable of giving a good description of the drying behaviour of wheat grains. The models found in the literature are based on dynamic equilibrium moisture contents. Probably the most well known equation is the one presented by O'Callaghan et al. (1971), which is of the Lewis type (Lewis 1921). Becker (1959) fitted the solution to the diffusion equation for spheres (approximated) to drying curves obtained from vacuum drying of wheat. Spencer (1969; 1972) used the coefficients derived by Becker

(1959) to simulate wheat drying in deep beds. To improve the agreement between the model and the experimental results, Spencer (1972) substituted an equation for dynamic emc (derived for maize) for the constant value of the approached moisture content used by Becker (1959).

8.2.1 *Mass-related drying rate*

Assuming that the internal resistance to moisture transfer is independent of particle size, the influence of particle size on drying rate is simple to model theoretically. The time required to dry particles of a specific shape is proportional to a power function of their masses ($m^{2/3}$). Assuming that the densities of the particles are identical, the relationship is valid for particles of any shape. Furthermore, the relationship is independent of whether or not the resistance to moisture transfer is a function of moisture content.

The Lewis equation (Lewis 1921) is the theoretical drying equation for particles whose resistance to mass transfer is concentrated in a thin layer at the outer surface of the particles. Assuming that the thickness of this layer is proportional to other dimensions of the particles, the influence of particle size on drying time is proportional to $m^{2/3}$. If the thickness of the layer is considered to be the same for all size particles, the drying time would instead be proportional to $m^{1/3}$. Since the concentrations of the components in different size kernels are similar (Paper IV), the former alternative of the two seems to be more realistic for grain kernels. However, models based on internal resistance to moisture transfer give a better description of the drying of cereal grains than the Lewis equation.

In order to analyze the influence of kernel mass on drying rate, kernels that had been stratified into narrow weight classes were rewetted to a moisture content of about 0.26 db and dried in thin layers at a nominal temperature of 60°C (Paper III). The kernel fractions were the same as those used in the study of the dimensional properties (two varieties). Fractions were exposed to the drying air for about 700 minutes. The drying curves obtained were fitted to different drying equations. Whenever applicable, the shape of the kernels was considered as spherical. For each variety, a long-term emc was experimentally determined; portions of the fractions containing the smallest kernels of each variety were dried at 60°C for about 84 hours.

To enable the different curves of a variety to be fitted to the drying equation collectively, the drying coefficient k was expressed in a mass dependent form (Eqn 3). Originally, k is defined as $\pi^2 D/r^2$, where D is the diffusivity and r is the radius of the drying particle. By optimizing the values of both the coefficients K and c in the fits (Eqn 3), the dependency on mass of the drying coefficient k was obtained in the coefficient c. This form of the relationship made allowance for the average shape of kernels to vary with the kernel mass. Other mass dependent coefficients in the drying equations were expressed analogously. Some drying equations examined contained two mass dependent coefficients. In these cases, two separate fits were made. In one of them the values of c were restricted to be the same for both coefficients, while individual values were allowed in the other.

$$k = Km^c \quad (3)$$

The values of c obtained in the fits varied between varieties. For the Avalon variety the values were about -0.65 for all equations fitted. This is close to the value (-2/3) that theoretically would be expected for particles of identical shape. The values obtained for the variety Kosack were higher and varied more between the equations. For the drying equations with best fit to data, the values of c were close to -0.45. This might be taken as an indication that while the shape of the Avalon kernels was independent of their mass, the sphericity of the Kosack kernels increased as their mass was reduced. However, the results of the analyses of the dimensional properties of the kernels show that this cannot be the case (Paper II). The dependence on mass varied less between the main dimensions of the Kosack kernels than between those of the Avalon kernels. While the sphericity and bulk density of the Kosack kernels were almost equal for all size kernels, the sphericity of the Avalon kernels increased with kernel mass. Furthermore, the visual appearance of the kernels supported the results of the dimensional analyses; small Avalon kernels seemed to be more angular than larger ones. Hence, the results of the dimensional study indicated that Kosack would be the variety for which the fitted c values should be closest to -2/3. For the Avalon variety, the fitted values of coefficient c should be lower than -2/3.

The two infinite series model was used to predict drying curves for 30 and 60 mg kernels of each variety Avalon and Kosack (Fig. 10). The maximum differences estimated between the moisture content of the two kernel sizes were 0.020 and 0.015 (db) for the kernels of Avalon and Kosack, respectively. At the times when the

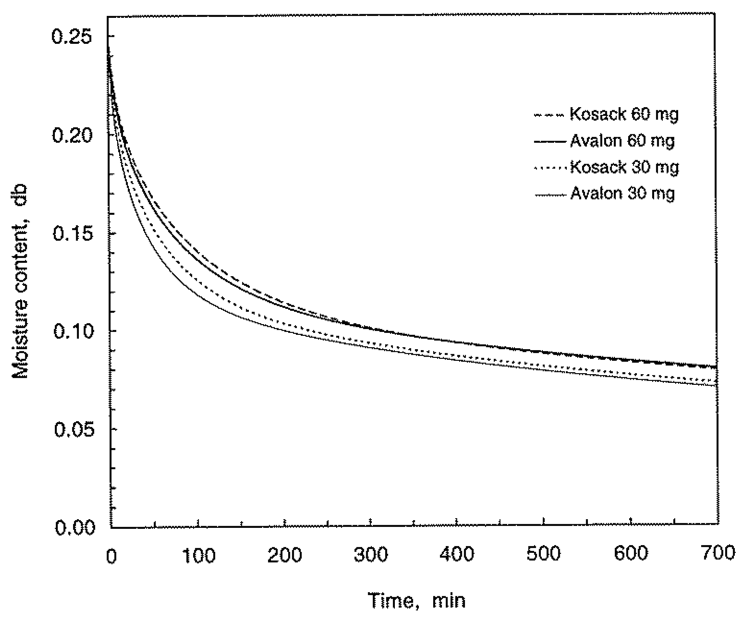

Fig. 10. Drying curves predicted for 30 mg (thin lines) and 60 mg (thick line) kernels of Avalon (whole) and Kosack (hatched) varieties by the two infinite series model. Individual values of c for the two drying coefficients.

maximum differences occurred, the moisture contents of the larger kernels were 0.158 and 0.154 (db) higher than the moisture contents of the smaller kernels of Avalon and Kosack varieties, respectively.

When individual values of *c* were fitted to the mass dependent coefficients in the drying equations containing two mass dependent coefficients, the obtained values of *c* differed between coefficients. The values of *c* obtained for the coefficients having their largest influence in the initial phase of the drying were lower than those obtained for the other coefficients. This indication of a higher dependence on kernel mass of the drying rate in the initial phase of drying, was supported by fits to the Page equation of truncated parts of the drying curves. The same tendency was obtained in the results of fits of truncated curves using the pseudo equilibrium moisture content presented by O´Callaghan et al. (1971). Using the long-term emc and truncating the curves at a moisture content of 0.16 db, the obtained values of *c* were -0.79 and -0.56 for the varieties Avalon and Kosack, respectively. Hence, the dependencies on mass of the drying rates expected from the kernel dimensions, were closer to the dependencies obtained for the initial parts of the curves, than they were to the dependencies obtained for total curves.

The difference between expected and obtained values of the coefficient *c*, was probably due to the drying models used not correctly reflecting the drying process in the kernels. Wheat grains are anisotropic. Their inner part, the endosperm, consists of relatively large starch granules which are imbedded in the intercellular protein matrix. The endosperm is surrounded by the aleuron layer and, outermost, the pericarp. To be able to model correctly the mass transfer inside a wheat kernel would therefore require knowledge of moisture transfer within and between the different components of the kernels. According to Brooker et al. (1992), Nagato et al. (1964) found that most of the moisture is evaporated in the region around the germ. Furthermore, in the drying models, all types of diffusion that might occur in a grain kernel are combined into a single term (Brooker et al. 1992). This might possibly explain why the relations between drying rate and kernel mass differed between the stages of drying process.

Thin layer models are used mainly as parts of larger models simulating the processes in dryers of various types. The accuracy of the drying models and the time required for using them (computational time) are both essential criteria when choosing between thin-layer models. Hence, the Lewis type equation (Lewis 1921) is probably still the equation type most commonly used in simulation models. The high rate of the increase in computational speed of personal computers will probably enable use of more cumbersome drying equations in future simulation models. Thus, it is still important to develop models capable of giving a good description of the diffusion process in the kernels under different conditions. This development should preferably include validations of the moisture profiles estimated within the kernels.

Internal moisture content profiles for a 40 mg Avalon kernel, predicted by the shell model, are plotted in Fig. 11. Due to the sharp breaks in the profiles predicted at the first nodal point inside the surface of the kernel, the estimates of first and second order derivatives are marred by errors in this nodal point. Increasing the number of shells in the model did not severely influence the parameters estimated. The break in the profile moved to the nodal point that became outermost of the internal nodal points. The trend

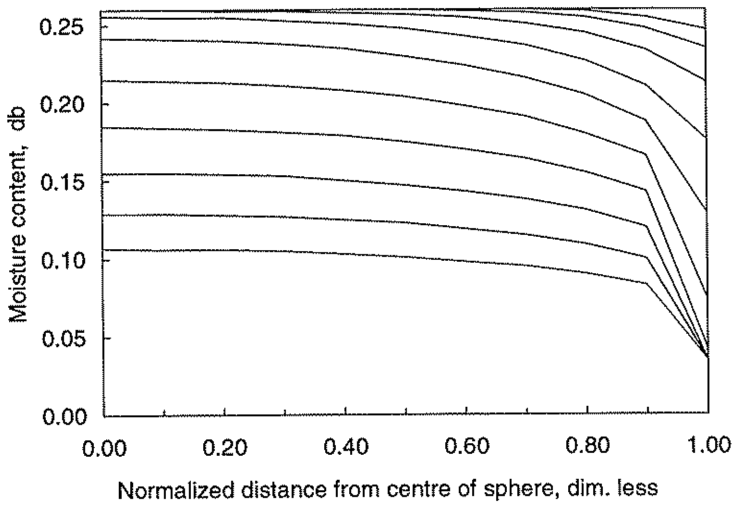

Fig. 11. Internal moisture content (db) profiles predicted for a 40 mg Avalon kernel by the shell model. Profiles within the spherical kernel are plotted at 1, 2, 4, 8, 15, 30, 60, 120, 240, and 480 min.

of the plotted profiles indicates that, apart from the outermost layer of the kernel where large moisture gradients exist, the moisture content varies only slightly with distance from the kernel centre.

Stroshine et al. (1986) dried thin layers of different hybrids of maize in air at 93°C. The time required to lower the moisture content from about 25 to 15% (wb) was used to compare the drying rates of the hybrids. Significant differences between the drying rates of the different hybrids were obtained. In 1980, the slowest-drying hybrid took 27% longer time to dry than the fastest one. The corresponding difference between the same hybrids was 42% in 1981. The varietal averages of drying rates did not correlate with the corresponding average masses of the kernels. For wheat, it has been stressed that the variation is low between varieties (Brooker et al. 1992).

The study (Paper III) revealed relationships between drying rate and kernel mass within two varieties of wheat. For both varieties, the dependency of mass was relatively close to that expected for different size particles of identical shape. However, the relatively large difference in drying rate obtained between the varieties in the study, implies that relationships between drying rate and kernel mass should not be expected to be valid between varieties. The drying rates of 40 mg kernels of the Avalon and Kosack variety differed by about 25% in the initial stage of drying (mc > 0.15 db). The varietal difference in drying rate might have been due to differences in the content, structure, or/and shape of the kernels. The visual appearance of the kernels suggests that the difference, at least partly, was caused by differences in the shape of kernels. Kosack kernels appeared to be rounder and to have smoother surfaces than Avalon ones. Thus, Kosack kernels should, at least initially, dry slower than kernels of the Avalon variety.

8.3 Content and quality of protein in wheat kernels

Loaf volume is considered to be the most important quality criterion for bread made of wheat flour. The better the bread-making quality of the flour the larger the volume of the bread baked from it. Although it is the complex of proteins called gluten that is primarily responsible for the exceptional characteristics of dough and bread made of wheat flour, even the total concentration of protein (nitrogen) in flour has been found to correlate well with loaf volume in many studies (Kent and Evers 1994). It is, nonetheless notable that there are other properties of flour than the content and quality of protein that exert an influence on its bread-making quality. For instance, excessive amount of the alpha-amylase enzyme in flour can ruin the bread-making quality of a flour, irrespective of its protein content.

About 95% of the wheat milled in Sweden is produced within the country. The remaining 5%, wheat with strong gluten characteristics, is imported mainly from Canada. Flour from the imported grain is blended into some of the domestic flours for production of the most quality-demanding products made by the baking industry. The amount of wheat that is imported depends on the quality of the domestic wheat grain, and therefore varies between years. Fractioning of domestic grain might possibly reduce the amount imported. With more differentiated qualities of the grain used in the milling industry, the grain used for the different flours could be better optimized. Wheat grain of low bread-making quality could be used for production of biscuit flour, or used as feed. Little is known about the variation in content of protein, or in the quality of the protein, among kernels in different wheat grain lots. To gain more knowledge about these variations the study reported in Paper IV was performed.

8.3.1 *Protein content*

The concentrations of protein (N*5.7) in kernels of four varieties of both spring and winter wheat were analyzed (Paper IV). The kernels were first sorted by mass into classes of narrow weight (1 mg). Then, the kernels in each mass fraction were stratified into two subfractions by their terminal velocity in air (aspiration). The lower the terminal velocity of a kernel, the lower the air flow required for carrying the kernel.

Within each spring variety, the concentration of protein increased with the mass of the kernels. Within the winter varieties, the concentrations were distributed differently among kernels, and the patterns of the distributions varied between varieties. Generally, for both spring and winter varieties, higher concentrations of protein were obtained for kernels with low terminal velocity than for kernels with higher terminal velocities. The concentration difference between the subfractions was dependent on the mass of the kernel; the larger the kernel the smaller the difference. The decrease in the concentration difference when kernel size increased was more pronounced for winter varieties than for spring ones.

Within the spring varieties, the relationships between protein concentration and kernel mass were similar to three of the five relations reported by Evans and Bhatt (1977) for Australian wheats. Dintzis et al. (1992), who used sieves to obtain different size classes, also reported that the concentrations of protein were higher among the larger kernels in most of the varieties they analyzed.

The concentrations of ash in the subfractions were also determined. Concentrations of ash were highly correlated to those of protein. The best-fit linear relationships between ash and protein concentrations accounted for 77 and 73% of total variations in ash concentrations within spring and winter varieties, respectively. The relative variation in concentration of protein was higher than the relative variation in concentration of ash.

A model was developed to estimate the variations in concentrations of ash and protein between kernels of identical mass. Within the fractions with the smallest kernels in each variety, the estimated variations were larger than the variations in the fraction averages within the corresponding varieties.

The large variations in the contents of ash and protein among kernels of identical mass were probably caused by differences in the degree of kernel filling (dilution with starch). This was indicated by the relationships between the contents of protein and ash in corresponding subfractions (Fig. 12). The appearance of the kernels supported the idea of attributing the degree of kernel filling to the large variations. Although kernels in all subfractions appeared normal and well-filled, the shape of the kernels in subfractions with the higher concentrations of protein and ash (low terminal velocity) were somewhat more angular than the shape of the kernels in the corresponding subfractions, when comparing them side by side.

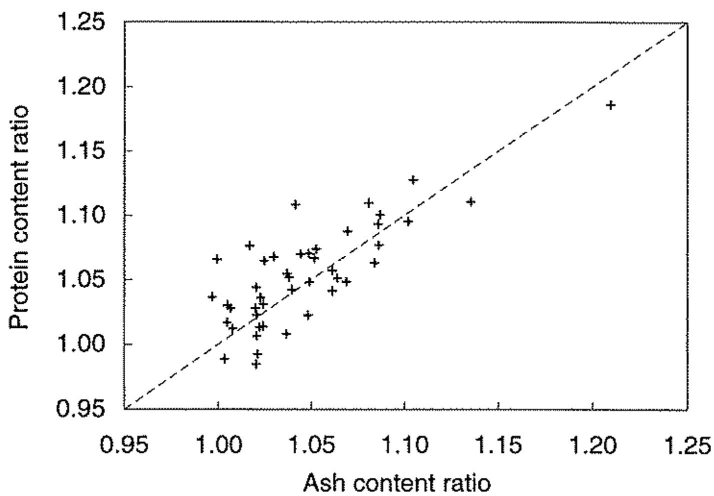

Fig. 12. Ratios between protein content in associated subfractions plotted against the corresponding ash content ratios. Hatched line represents the relationship 1:1.

8.3.2 *Protein quality*

The bread-making quality of a flour can be estimated on the basis of several methods. The Zeleny (Zeleny 1947) and SDS sedimentation tests (Axford et al. 1979), and the gluten index method (Perten 1989) are examples of methods used to estimate the value for baking of the protein components in flour or/and meal. Some instruments, as the Farinograph, the Extensograph, and the Alveograph, estimate bread-making qualities by the rheological properties of dough. However, none of these methods can give a good prediction of the baking result in all situations.

The SDS sedimentation test and the gluten index method were used to estimate the quality of protein in the subfraction meals. Four varieties (two winter and two spring) were subjected to the SDS sedimentation test. The subfraction meals of the other four varieties, were analyzed for their gluten content (wet) and gluten index. Each of these methods requires only a small amount of grain, and permits the use of meal instead of flour.

The SDS volumes increased with the mass of the kernels within the spring varieties (Fig. 13). In one of the spring varieties, the SDS volumes for the subfractions of the largest kernels approached the maximum of 100 ml. Although the protein contents generally differed significantly between kernels of the different types of subfractions, similar SDS volumes were obtained for the corresponding subfractions. Within the winter varieties, the SDS volumes varied less between subfractions. The differences in SDS volumes were lower than what could be expected from the protein contents in the corresponding subfractions, at least among the subfractions of low kernel masses. Hence, SDS volumes seem less dependent on degree of kernel filling than do protein contents.

Johnson et al. (1975) found that the degree of kernel filling strongly affected the protein contents. Krattinger and Law (1991) concluded, on the basis of their own studies and the work of others, that at low protein contents (less than 13%) the SDS volume is correlated strongly and positively with protein content and other quality parameters, whereas at higher protein contents the correlations tend to be negative and/or non-significant. The fact that the relation between SDS volumes and protein contents

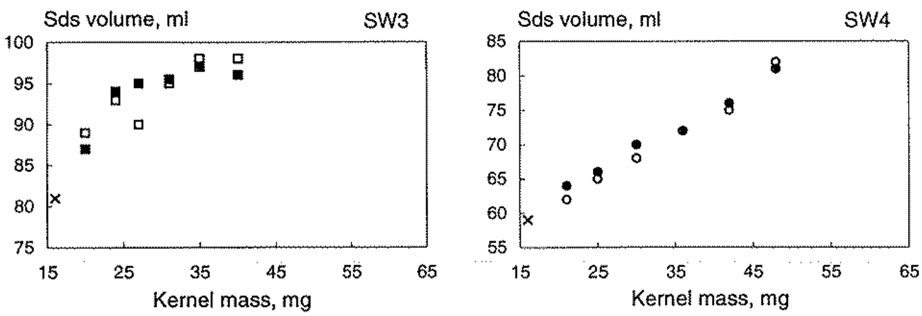

Fig. 13. SDS volumes for kernel-mass subfractions of two spring wheat varieties. Filled and unfilled symbols represent kernels of high and low terminal velocity, respectively. x represents not sorted fractions.

varied with the degree of kernel filling (Paper IV) could be a possible explanation of the dependence on protein content of the relationship between SDS volume and protein content.

At a given content of protein, the wet gluten content tended to be higher for kernel subfractions with high terminal velocities, than for those with low terminal velocities. This is another indication of protein (nitrogen) in less filled kernels having a lower value for baking than the protein in more plump kernels.

Gluten index is a measure of certain gluten strength characteristics (Perten 1989). The index has been found to give good prediction of the quality of durum flour and semolina for pasta-making (Cubadda et al. 1992). Because the bread-making quality of a flour is not solely dependent on gluten strength, a correlation between gluten index alone and bread-making qualities cannot be expected (Perten et al. 1992). However, Rychener and Tièche (1993) obtained relatively good correlations between gluten index and some other bread-making quality measures. The statistical analysis was based on 220 samples of a single wheat variety (two years). The fact that gluten index values correlated with the other measures was probably due to the relationship obtained by Rychener and Tièche (1993) each year between the gluten index and gluten content. Also Perten et al. (1992) obtained within-variety relationships between the gluten index and gluten content. The higher the gluten content the lower the gluten index. Perten et al. (1992) suggested that location, climate, soil conditions or fertilization could each have contributed to determining the relation obtained.

Within each of the four varieties analyzed, the gluten index of the meals decreased as the mass increased of the kernels from which it was ground. Index values were much lower for the subfractions of winter varieties than they were for subfractions of spring ones. For the spring varieties, the index values correlated inversely with gluten content. The slope of each varietal relationship was similar to the slope of the relationship obtained by Perten et al. (1992) for different samples of variety Kosack. The slopes of the relationships obtained by Rychener and Tièche (1993) were different, probably being a result of a few samples in their investigation deviating from the major trend. The strong varietal relationships between gluten index and gluten content could be taken as an indication that they vary with each other in a predetermined way. However, we earlier found (Regnér *unpublished*) that delayed harvest could increase the index values without any corresponding changes occurring in the gluten content.

The general differences between the spring and winter varieties in their mass-related distributions of protein content, ash content, and protein quality measures might have been determined by genetic or/and environmental factors. Spring and winter varieties were grown at different locations, and the winter varieties showed higher levels of pathogen infection. Differences in typical configurations of kernels within ears, and in degree of tillering within stands might also have influenced the mass-related distributions of the properties analyzed. To ascertain whether the results are typical for winter and spring varieties, more studies have to be performed.

If we can suppose that the mass-related distributions obtained in this study are typical of the two main types of wheat, the sorting of spring wheat grain lots would be far more interesting than sorting of winter ones. According to the SDS volumes for the subfractions of spring wheats (Fig. 13), the kernels with the highest masses would be those that are most suitable for bread-making.

Using the measures obtained by the gluten index method to compare the value for baking of the protein components in the subfractions, both the gluten content and the gluten index value should be considered. Perten Instruments AB, marketing the equipment used for the gluten index method, stresses that for bread-baking and at a given gluten content, the optimum value of the gluten index is between 60 and 90 depending on baking method and type of bread. Using some relationships revealed in other studies between the baking quality and the two gluten measures (Nilsson and von Koenigsmarck 1994), bread volumes were estimated for the subfractions in this study. For the spring varieties, the predicted bread volumes increased with the mass of the kernels. A positive relationship between the estimated bread volume and kernel mass was also found in one of the winter varieties (WW1). Within the other winter variety (WW2) analyzed, the predicted bread volumes were inversely related to the mass of the kernels. The differences between the estimates for the two subfraction types were relatively small compared with the dependence on mass of the estimated bread volumes.

The protein content in meal has been found to correlate highly to that in flour (Vogel et al. 1976, Sylvester-Bradley 1990). For the corresponding relationships between meal and flour gluten contents, and between meal and flour gluten index values, Perten et al. (1992) obtained good correlations (r=0.97 in both cases). These good correlations indicate that similar relationships between contents and quality measures would have been obtained within the varieties even if the subfractions had been milled instead of ground. Then the results should be applicable also to differences in flour properties.

8.4 Ergosterol content in relation to kernel mass

Fungi are the most important spoilage organisms in cereal grains. They may severely reduce the value of the grain, both in the field and in storage. Fungal growth affects cereal grains mainly by heating and development of mustiness, potential production of toxins, dry matter losses, biochemical changes, discolouration, and decreases in the germinability (Lacey and Magan 1991, Brooker et al. 1992, Börjesson 1993). Effects of storage conditions on fungal growth have been focused in many studies, especially moisture (water activity), temperature and the gaseous atmosphere (Lacey and Magan 1991). Plant pathologists have often investigated the effects of specific fungal diseases in field, such as *Fusarium culmorum*, on yield and kernel weight (Snijders and Perkowski 1990).

Several criteria are used to compare grain samples on the basis of their microbiological status; presence of visible mould, number and types of mould colony-forming units, production of carbon dioxide, grain odour, and content of ergosterol, are examples of such criteria. The content of ergosterol, and the concentration increase in this component are promising criteria for assessing the quality and storability of grain (Brooker et al. 1992, Schnürer and Johnsson 1992).

Ergosterol appears exclusively in fungal membranes (Weete 1980), and is commonly used as a marker of fungal growth in grains (Seitz et al. 1977, Young et al. 1984, Müller and Lehn 1988, Schnürer and Johnsson 1992). Young et al. (1984) found 85-90% of the total content of ergosterol in the bran fraction, after milling soft wheat. The conclusion that the highest concentrations of ergosterol are found in the outer layers of the kernels, was supported by the results of a study of Schnürer (1991). In this, only 3% of the total ergosterol content was obtained in flour, whereas fine and coarse bran accounted for 43 and 54%, respectively.

To investigate if the concentration of ergosterol in grain kernels varies with their masses, the kernels in each of five lots of different winter grain varieties (three wheat, one rye, and one triticale) were stratified by mass (Paper V). Particles that were not classified as whole, sound kernels were, for each variety, combined into an impurity sample also analyzed for ergosterol concentration.

After the harvest of the field trial plots the grain lots obtained were dried in slightly heated air to a moisture content of about 14% (wb). Before analyzing them, they were kept at a temperature of about 10°C. Due to adequate drying and storage, the ergosterol contents obtained in analyses were attributed more to infections in the field than to fungal growth occuring later.

Within each variety, the ergosterol concentrations decreased as the mass of the kernels increased. This result was expected because of the high concentrations of ergosterol in outer layers of the kernels, and due to the surface to volume ratio decreasing as the size of the kernels increases. A physically based model (Eqn 4) was developed to examine if the obtained relations between ergosterol concentrations (A') and kernel masses (m) could be explained by the surface to volume ratios of the kernels. The value fitted to the coefficient f (c_2 in Paper V) should indicate whether or not the degree of infection was constant per unit surface area of the kernels. For identically shaped three-dimensional bodies of different size, the expected value of f would be 3.0 if the degree of infection on the kernel surfaces was the same. The corresponding values for infinitely long cylinders and infinite plates would be 2.0 and 1.0, respectively. Because the length was found to vary less with size than the other kernel dimensions (Paper II), a value slightly lower than 3.0 would be expected for grain kernels. The value of the coefficient d is determined by the degree of infection.

$$A' = dm^{-\frac{1}{f}} = de^{-\frac{1}{f}\ln(m)} \qquad (4)$$

For four of the five varieties, the fitted values of the coefficient f ranged from 0.39 to 0.86. For the rye variety, the best fit value of f was 2.76.

Only the variation in the ergosterol concentrations within the rye variety could be explained by the surface to volume ratios of the kernels. The low values of f obtained for the wheat and triticale varieties indicate a shape of the kernels for which the absolute surface area increases as size is reduced. Obviously this is not true. Hence, the degree of infection per unit surface area of the kernels was much higher for small kernels than it was for larger ones. For the kernels of the wheat and triticale varieties, not only the concentrations but also the absolute content of ergosterol increased as kernel size decreased.

Based on the low levels of fungal infection in the field, the normal appearance of the mass distributions, and the effects of fungal infections on kernel mass found earlier (Section 7.3) it was considered improbable that small kernels were small because of their high levels of infection. Instead, the higher degree of infection on small kernels might have been due to size-related differences in average climatic conditions to which the kernels were exposed. Within spikelets of wheat and triticale, the larger kernels are situated at both ends, whereas smaller kernels are pressed between the larger ones. Size-related differences are also found between the kernels in different ears in the crop. Ears on tillers of high orders contain kernels of lower masses and are usually found deeper in the stand (Dahlstedt 1985). Thus, the somewhat larger kernels in the main ears are better ventilated and might therefore become less infected than the corresponding kernels in ears of higher order tillers.

That the distributions of ergosterol concentrations differed between rye and other varieties might have been due to the average climatic conditions to which the different size kernels were exposed being more uniform for rye than they were for wheat and triticale. The configuration of the kernels in rye ears differs from those in wheat and triticale; while seldom more than two kernels develop in the rye spikelets, up to five kernels of different size develop in those of wheat. Another difference between the species is that at the end of the growing season, the kernels in ears of wheat and triticale are normally well hidden in the spikelets, whereas the kernels of rye are more exposed. However, since only one sample each of rye and triticale was analyzed, the differences identified here between rye and the others might not be species-specific.

Bechtel et al. (1985) assigned winter wheat kernels infected with *Fusarium graminearum* to one of three categories, based on appearance: 1) kernels appearing sound and of good colour and weight; 2) lightly infected kernels of normal size but of light weight and colour; and 3) heavily infected kernels that were shrivelled and light-coloured. The 1000-kernel weights of the kernels in the three categories were 29.9, 25.6, and 13.1 g, respectively. The concentrations of ergosterol in the fractions were 2.8, 29.0, 103.0 ppm. Thus, the degree of infection per unit surface area varied with kernel size also in this study. However, the rate of the increase in ergosterol concentration as mass decreased was higher in the study of Bechtel et al. (1985) than in the one reported in Paper V. This might be due to the fact that the degree of infection, and thereby the appearance, varied highly among kernels of the same masses. This would be in line with the contents of ash and protein in kernels (Paper IV).

For each grain lot, the ergosterol concentration in the impurities was much higher than the average concentration of the kernels. Similar results were obtained by Seitz et al. (1986) in a study of the effectiveness of different cleaning methods to lower the content of deoxynivalenol (DON), a metabolite of *Fusarium graminearum*, in the grain.

Due to the relatively low mass of impurities and small kernels, removal of these components would not influence significantly the concentration of ergosterol in the remaining grain. However, if there were significant concentration differences between kernels of identical mass, aspiration of sieved fractions might better sort kernels in accordance with their individual levels of infection.

8.5 Malt extract yield - kernel mass

In Europe, the production of malt is normally based on two-rowed barley grains (Kent and Evers 1994). In the malting process cereal starch is converted to soluble sugars. Since higher concentrations of starch are normally found in well-filled, large barley kernels, the malting industry prefers these to smaller ones. In addition, the kernels should be of uniform size since the time required for the physical modification in the kernels is size-dependent. Partially modified kernels not only give low extract yields, they also release soluble beta-glucans in the mash, which cause problems in the process (Seward 1992). On the other hand, over-modification may adversely affect properties of the beer (beer foam, flavour, and shelf life).

The dependence on kernel size of extract yield was investigated in a minor study (Regnér *unpublished*). Barley kernels of variety Meltan were stratified by mass into classes of narrow widths. Some of the kernel fractions were further sorted by sieving (2.8 mm wide, oblong holes). The fractions obtained were steeped in a Carlberg micro-malting unit (Danbrew, Copenhagen, Denmark) at 16°C (5 h wet, 15 h dry, and 8h wet). Kernels were germinated for 120 hours (12°C) and the kilning was done in three stages (10 h, 50°C; 8 h, 60°C; and 8 h, 80°C). The samples were ground in an DLFU disc-mill (Bühler-Miag GmbH, Braunschweig, BRD) with a spacing of 1.0 mm between plates. Mashing and filtration were done in accordance with Analytica-EBC (1987). The extract yields were determined with a refractometer (Abbemat-HP, Dr Wolfgang Kernchen GmbH, Seelze, BRD). A Beta-glucan 5700 Analyzer (Tecator, Höganäs, Sweden) was used for determining the concentrations of beta-glucans.

At low kernel masses (<50 mg), the extract yield increased with the mass of the kernels (Fig 14). However, at kernel masses above 50 mg, the extract yield correlated inversely with the mass of kernels. In three of the four mass fractions that were sifted, higher extract yields were obtained for subfractions of kernels that did not pass through the sieve than were obtained for those passing the screen. Thus, both the size and shape of kernels influenced the extract yield.

The relatively low extract yields of the fractions containing the largest kernels was probably because these kernels were only partly modified. If the large kernels had been allowed to germinate for a longer period this would probably have increased the extract yields of these kernels. Another possible explanation of the relationship obtained would be that the concentrations of starch were not highest among the largest kernels. At least for some of the winter wheat varieties analyzed in Paper IV, the concentration of starch would be expected to have an optimum at an intermediate kernel mass.

In Fig. 15, the concentrations of beta-glucans in the extracts of the different kernel fractions are presented. The overall trend of the plotted data is that the concentration of beta-glucans increases with the mass of the kernels. However, disregarding the concentration obtained for the fraction of the largest kernels, it seems that also the concentration of beta-glucans would be highest for kernels with masses of about 50 mg. The higher concentration obtained for the disregarded fraction could be explained by the time-dependent development of beta-glucanases. This enzyme develops in a late stage of the germination process and reduces the amount of beta-glucans (Seward 1992).

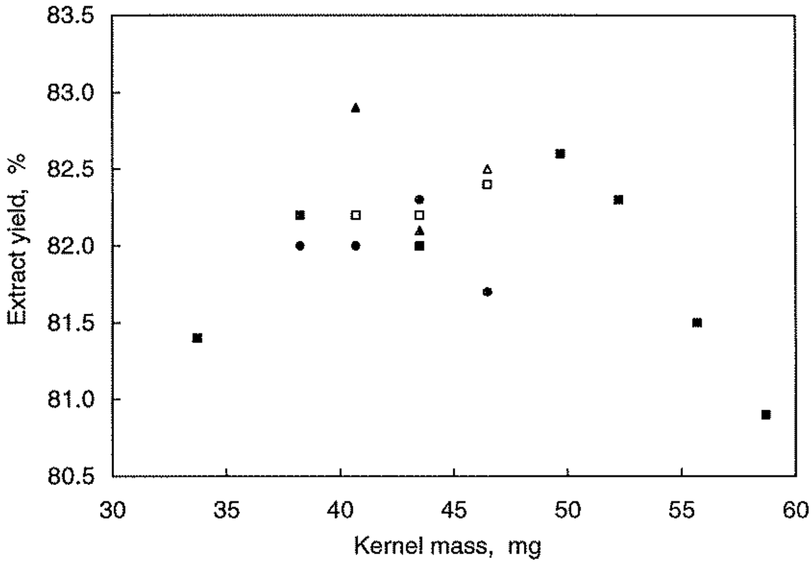

Fig. 14. Extract yields for mass fraction (squares) and for subfractions passsing the screen (triangles) and for those that did not pass (circles) the screen. Filled and unfilled symbols represent measured and calculated values, respectively.

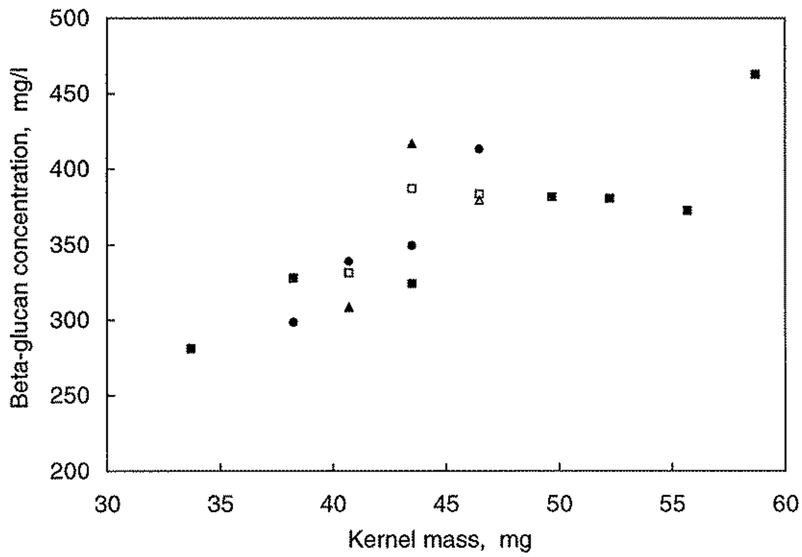

Fig. 15. Concentrations of beta-glucans in mass fraction (squares) and in subfractions passsing the screen (triangles) and in those that did not pass (circles) the screen. Filled and unfilled symbols represent values measured and calculated, respectively.

9. GENERAL CONCLUSIONS

The system developed determines distributions of mass automatically, and therefore enables weighing of large numbers of kernels. This is essential for the confidence of the statistical measures calculated for the distributions, and, hence, for comparisons of these between samples. For the examined samples of wheat, rye, triticale and six-rowed barley varieties the relative variations in mass (coefficient of variation) ranged from about 20 to 30%. The corresponding degrees of variation obtained for the two-rowed barley varieties were about 15%. For oats, the distributions contained two peaks, each of relatively low width.

Subjecting samples representing different treatments in the field to determination of mass distribution, the graphically presented distributions and the statistical measures describing them can be used to analyze closely the influence of different treatments on kernel growth. This was found to be a suitable method for studying the effects of fungicide use on the growth of different size kernels. The obtained knowledge of kernel mass variations was used to analyze the reliability of average kernel masses, estimated for grain lots, in relation to the number of kernels that were measured.

The ability of the system to sort kernels by mass was found to be an excellent tool for gaining knowledge of the variations in kernel properties within grain lots. The dependence on mass of a kernel property is determined directly through analyses of the obtained fractions. The variation in the property can also be determined in other dimensions. Then, kernels of identical mass are sorted by other properties than mass. The revealed relationships can serve as a basis for how grain lots should be sorted to optimize the use of grain. Internal relationships can also be a suitable basis for studies of variations between different stands. Hence, the system is useful as a tool for researchers in studies concerning the development of stands.

In the thesis, the potential for sorting kernels by mass was exemplified in studies focused on dimensions of wheat kernels, drying characteristics of wheat grains, content and quality of protein in wheat, kernel ergosterol concentrations, and malting properties of barley grains.

Because the grain samples used in each study most often originated from a few varieties, grown in a single year and at the same location, the results obtained should be used with care. More investigations are needed to validate the relationships revealed in the studies.

9.1 Future research

In this thesis, the usefulness of the system has been exemplified in a number of studies. Knowledge of the internal distribution among kernels is of interest for many other properties of cereal grains. The activity of alpha-amylases in different kernels and the reduction of the activity in grain aimed for baking are, for example, of great importance for the milling industry. The properties of the starch in different types of kernels is another interesting field for future research.

Some of the results of the studies reported in the thesis open up routes for further investigations based on the system developed:

The relationships between protein quality and kernel mass, particularly within spring wheat varieties, are worth further study. Such a study should include validations of the relationships described in Paper IV, and should focus on the use of conventional sorting equipment to stratify kernels into fractions of different bread-making qualities. Furthermore, it should be validated that the quality estimated for different sized kernels corresponds to true bread-making qualities.

The effect of size and shape of kernels on the extract yield and concentration of beta-glucans should be further investigated. The time allowed for the physical modification could be optimized based on the time and size dependency of extract yield and of the concentration of beta-glucans. Then also the effect of grain fractioning before malting could be modelled.

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