Models for Internal Quality Fruit Sorting, Based on Time-Domain Laser Reflectance Spectroscopy (TDRS)

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1. Abstract

Time domain laser reflectance spectroscopy (TDRS) was applied for the first time to evaluate internal fruit quality. This technique, known in medicine-related knowledge areas, has not been used before in agricultural or food research. It allows the simultaneous non-destructive measuring of two optical characteristics of the tissues: light scattering and absorption. Models to measure firmness, sugar & acid contents in kiwifruit, tomato, apple, peach, nectarine and other fruits were built using sequential statistical techniques: principal component analysis, multiple stepwise linear regression, clustering and discriminant analysis. Consistent correlations were established between the two parameters measured with TDRS, i.e. absorption & transport scattering coefficients, with chemical constituents (sugars and acids) and firmness, respectively. Classification models were built to sort fruits into three quality grades, according to their firmness, soluble solids and acidity.

2. Introduction

Non-destructive measurement of fruit quality has been a primary and widely established research objective along the past years (Abbott 1999; Chen *et al.* 1991; Hakim *et al.* 1999).

Many different techniques have been developed and applied to create sensors to measure quality parameters. Generally speaking, some of them are oriented to the detection of physical aspects of the samples (i.e. firmness, presence of holes, seeds, skin colour, size/shape, defects, etc.) and the rest are focused on chemical detection (i.e. quantify main components, residues, etc.)

One of the limitations of these techniques consists in the fact that they can only detect one quality property, so they have to be combined with other sensors if we want to use them to obtain a more complete information on fruit quality. Among them, the techniques based on optical properties of tissues and chemicals, and the interaction between radiation and matter have been proven useful in many research labs (Bellon *et al.* 1993; Jordan *et al.* 1997; Kawano 1994; Moons *et al.* 1997; Gunasekaran *et al.* 1984).

2.1. Review/comparison with other NIR techniques

Near infrared spectroscopy (NIR) is known traditionally for its applicability to the quantification of internal chemicals of foods (Lammertyn *et al.* 1998; Yantarasri *et al.* 1997). NIR absorption is based on the Lambert-Beer principle ($A=\ln [I_0/I]$) and can be easily converted into transmission. However sometimes, as in our experiment, is more advantageous to work with the NIR equipment in a "reflectance set-up". In this case, the re-emitted light is collected out of the sample after passing through a portion of it. This way of measurement is often called "body reflectance" (Chen *et al.* 1980).

Furthermore, the main limitation of the techniques that measure light transmission properties of matter is that they do not account for the coupling between absorption and scattering inside the tissue, when quantifying the intensity of re-emitted light. This means that it is not possible to measure intensity of absorption without having its value affected by the effect of scattering. This is why it is not immediate to obtain quantitative information of absorption and scattering independently with one local measurement of total reflected light, and at a time. This paper describes how the TDRS technique is capable of doing so.

Most commonly used light sources in NIR equipment are the tungsten lamps, which provide a satisfactory spectrum over VIS & NIR. Nevertheless, some trials have been done (Martin *et al.* 1996; Tu *et al.* 1995) with more powerful, monochromatic light sources like the lasers. In spite of the theoretical disadvantage of a laser system, which is not appropriate to acquire broad spectra, their use presents unique characteristics, like the ability to be precisely adjusted and its coherent behaviour. Indeed, it has been noticed that NIR laser "spectroscopy" can be used to estimate the firmness of the fruits (McGlone *et al.* 1997) although is has not been tested much further.

On the other hand, usually to implement any NIR spectroscopic technique, specific wavelengths or narrow windows are identified as the most correlated ones with different chemical compounds, and a different area along the spectrum could be used to extract firmness information. Even though this is an advantageous set-up for the development of a sensor (it will be able to obtain more than one quality parameter at a time) the final equipment will have to cover a wide range of wavelengths, some for the chemical and some for the firmness estimations respectively.

Our technique, TDRS or TRR (time-domain reflectance spectroscopy or *time resolved reflectance*) will use only a reduced number of laser wavelengths, obtaining information both on chemical composition of the tissue and on firmness, using the same wavelengths. This is feasible because this technique uses a property of light-matter interaction that has not been applied before on the measurement of fresh food properties: it measures the time that light needs to be injected, pass through and reach out the fruit, and the amount of it.

The objectives of the experiments carried out within this work were:

1. To study the applicability of a new optical technique, TDRS, to measure internal fruit quality non-destructively (firmness, sugars and acids)
2. To build up fruit quality estimation models based on TDRS parameters, and test their performance

To achieve these objectives, it is necessary to measure a large amount of samples to build up a representative database to study the links between the optical TDRS parameters and the standard destructive test, and then to carry out modelling for the adjustment of such links between the TDRS variables and the fruit quality parameters, for each species of fruit.

Notation

Variables	meaning	Variables	meaning
MA600 ...MA1000	TDRS absorption coefficient, μ_a, at each wavelength (600 – 1000nm)	MTF1	Max force during Magness-Taylor test, N
MS600 ...MS1000	TDRS transport scattering coefficient, μ'_s, at each wavelength (600 – 1000nm)	MTD1	Deformation at max force during Magness-Taylor test, mm
C400 ... C700	VIS reflectance, % (skin colour)	MTG	Gradient (slope) of the curve during Magness-Taylor test, N/mm
BF1	Max force during compression with ball test, N	PF1	Max force during puncture with needle test, N
BD1	Deformation at max force during compression with ball test, mm	PA1	Area below curve (absorbed energy) during puncture with needle test, mm^2
BFD1	Ratio max force/deformation (slope) during compression with ball test, N/mm	PT	Max deformation (travel) during puncture with needle test, mm
BA1	Area below curve (absorbed energy) during compression with ball test, mm^2	PG	Gradient (slope) of the curve during puncture with needle test, N/mm
BT	Max deformation (travel) during compression with ball test, mm	ACID	Total acidity of squeezed juice, meq/l
SUGAR	Soluble solid content, °Brix	BATCH	Number of fruit batch
DAY	Day of measurement	FRUITN	Fruit number inside batch

3. Procedures

3.1. Description of the TDRS fundamentals

The TDRS or TRR (time-domain resolved spectroscopy or time reflectance spectroscopy) is based on the measurement of the broadening of a short light pulse, transmitted across a turbid medium (fruit tissues). The light source is a laser beam, monochromatic then, but tuneable at several wavelengths. The light is injected in the fruit through the intact skin by means of fibre optics positioned perpendicularly to the equator of the fruit. The light flux crosses the tissues and part of it finds its way out of the sample at a particular region adjacent to the

injection point. This portion of reflected light was recovered with other fibre optics placed at about 20 mm in parallel to the injection ones. The three-dimensional light region formed by the light which is capable of entering the recovering fibres is commonly named "banana" after the shape that is constructed by the optical paths of the photons with larger probability of being recovered after suffering internal reflection. If an adequate theoretical model is used for the experimental analysis of data and several hypothesis are established, it is possible to calculate at the same time the absorption coefficient and the transport scattering coefficient at each wavelength, with good precision.

The TDRS equipment used in these work is described in detail in the following references: (Cubeddu *et al.* 1994a; Cubeddu *et al.* 1994b; Cubeddu *et al.* 1999)

This technique has been developed for use in the field of medicine, for the detection of discontinuities in tissues and the location of human tumours. In this work the objective was to apply time-domain resolved reflectance spectroscopy for the characterisation of the optical properties of selected fruits, which can be used for the non-destructive internal evaluation of several aspects of fruit quality.

3.2. Plant material: sampled fruits , campaigns

Along three years (1996, 1997 & 1998) several experimental campaigns have been held by the UPM research group in close co-operation with the Physics Dept. at the Politecnico di Milano, at their Milan facilities. These measurements were planned to cover a wide range of samples, fruit species and maturity stages. The material sampled for this collaborative measurements was entirely acquired at the local markets of Milan, during the different measurement periods (February, July & November). It was selected piece by piece to obtain, concerning to quality parameters, higher variance between batches than inside each one of them. Apples, peaches, kiwis, and tomatoes have been measured at different moments,

conforming a wide database of optical and destructive parameters. Taking into account all measurements: the firmness ranges are 30N (max force Mg-Ty) for apple, 60N for peach, 4N/mm (force/deform in puncture) for kiwi, and 2N/mm for tomato; the sugar ranges are 8 °Brix in apple, 4°Brix in peach, 4°Brix in kiwi and 2°Brix in tomato; the acidity ranges are 78meq/l in apple, 74meq/l in peach, 61meq/l in kiwi and 31meq/l in tomato.

3.3. *Measurements and protocols*

The physical and chemical essays done on each fruit are summarised in table 2. On each fruit, a selection of two sides was made, choosing as side 'A' the most coloured side, and side 'B' the opposite side. Further data analysis was done on the average value for the whole individual fruit.

To characterise the physical state of the samples, several tests could be applied to the fruit, which are able to typify different mechanical aspects (Barreiro *et al.* 1997). In this case, the selected mechanical tests were:

Puncture of fruits (tomatoes and kiwis). It was carried out with a Texture Analyser machine, model TAXT2, with a cylindrical probe of 0.8 mm diameter and flat base. It was applied through the skin at 20mm/min speed rate, up to 8 mm deep. Deformation was immediately removed at the same speed rate; one repetition was made per side of each fruit. The following parameters were registered through this test: maximum force (N), maximum deformation (mm), ratio force/deformation (N/mm) at max puncture force, area below curve (mm^2) (see notation table for acronyms).

Magness-Taylor penetration of the flesh (apples and peaches). Carried out with the Texture Analyser, each sample side was peeled and pressed with the metallic cylinder (8mm of diameter and rounded head). Two measurements were done per fruit, one on each side. The penetration was done at a speed rate of 20mm/min and stopped when 8 mm of deformation was achieved. Maximum force (N), maximum deformation (mm), and ratio force/deformation (N/mm) were registered (see notation table).

Quasi-static compression with sphere (kiwis). Also carried out with the Texture Analyser, each fruit was tested by compressing it on the skin with a steel sphere of 19.5 mm diameter. It was done at a speed rate of 20 mm/min and stopped when 3 mm of deformation was achieved ; two measurements on each fruit, one per side. The parameters registered were maximum force (N), maximum deformation (mm), ratio force/deformation (N/mm), and area below curve (mm^2) (see notation table).

Chemical tests were also carried out on the samples:

Titration of total acid content. It was done in a different way in apples, peaches & kiwis than in tomatoes: For this last one, the external part (pericarp and outer mesocarp) was separated from the internal part (loculi, liquids and seeds), so four measurements for each tomato were taken (two sides x two parts). After extracting the juice from each part, a known volume of it was filtrated and titrated with a solution of sodium hydroxide. The milliequivalents of acid concentration were calculated for each fruit.

Refractometric index. Brix degrees (soluble solids content) were measured on both sides from the juice of the samples, using a digital refractometer. In the case of tomatoes, four measurements were distinguished also.

3.4. Statistical analysis process

Based on previous experience on data analysis and model creation (Ruiz-Altisent *et al.* 1994), a complex statistical process has been followed along three years, consisting of three steps:

1st Step. Using Principal Component Analysis (PCA) and Multiple Stepwise Linear Regression (MSLR), the relations between the different measurements were searched for.

2nd Step. Clustering techniques were used to "naturally group" fruits according to their quality.

3rd Step. Discriminant Analysis (DA) was the tool to build the models for firmness, sugar and acid content estimation.

4. Results

4.1. Performance of the TDRS technique

Some observations about the technique can be done. The depth that the light goes into the tissue was measured and it is about 1 cm deep into a thin-skinned fruit, as an apple. Therefore, the quality attributes measured by the TDRS correspond only to a portion of fruit flesh contained in the correspondent volume which, in many cases, can be a good representation of a fruit, or of a half fruit. As two measurements were done, one for each side, and then averaged, stable conclusions can be established for the whole fruit.

The acquisition time for each TDRS measurement takes 3 seconds approximately. As the whole measuring device is computerised and the light pulses are short (in the pico-second order of magnitude), the signal acquisition and processing depends only on the electronic board performance and on the operator skills to place the fruit.

4.2. 1st step: PCA, MLR

A fruit is a very complex body, and no simple correlations exist between light absorption, scattering and macroscopic quality parameters. As the main objective at this stage of the project is the evaluation of the TDRS as a useful technique to test quality parameters on fruits, a large statistical process has been needed to identify the links among optical data and destructive tests. In this paper, we have tried to extract the main conclusions of the analysis are presented.

A database was built joining the data obtained from the standard destructive techniques with the data collected with the TDRS equipment. For the subsequent statistical analysis, the average of both measurements on each side of the fruit (A and B) was considered an independent measurement.

At the first step, to search for initial correlation between the TDRS, and the measurements of firmness, acidity and sugar, the Principal Component Analysis and Multiple Stepwise Linear Regression techniques were used.

Initially, the PCA were carried out including all the measurements and variables together. In table 3, there are the summaries of these analyses, with the first two factors extracted out of each PCA. With this approach, the first remarkable result was that all the variables incorporated were explaining only 30% of the total variance contained in the database. This fact may indicate that the true links between the TDRS light behaviour inside the fruit and their quality are still unknown, and depend on uncontrolled sources of variation, not taken into account in these experiments.

Also, the results of these PCAs were conditioned by the amount of variables introduced in them, belonging to specific information groups; for example, if too many VIS reflectance variables are included, compared to the chemical content variables, the results are biased to the "colour information". Nevertheless, some trends could be traced and the correlations found in the first PCAs were validated with newer PCAs (not shown), particularised for each specie and each type of relation between variables: firmness with TDRS scattering, and chemical contents with NIR absorption.

The results for each kind of fruit are :

Peach: Considering all the measurements together, without distinction of variety type, side or batch, it was seen that, with the PCA, most of the firmness variables showed clear correlation (R^2>0.75) with the scattering at 750 and higher. When building up MLR models with the laser variables to predict firmness (Magness-Taylor slope) the estimation was almost equal when including absorption and scattering variables (R^2=0.67) than when using only scattering ones (R^2=0.63). The TDRS variables in the NIR region presented good correlation (R^2>0.8) with chemical compounds.

Kiwi: In the first approach, with all the measurements together, the Principal Component Analysis (PCA) showed clear correlation (>0.75) between firmness variables (puncture : force, slope, etc.), and scattering at 670nm, 750 and higher. It was noticeable some correlation between sugar content and scattering, linked also with firmness; this fact was not seen in other fruits.

Apple: In an analogous way, considering all the measurements together, it was found a clear correlation (from 0.7 to 0.9) between many firmness variables (load/unload of probe and Magness-Taylor) and laser scattering variables (at 675, 750 and 800nm). Sugars and acids were correlated with TDRS NIR wavelengths with scores reaching 0.8.

Tomato: As in the other case, considering all the measurements together, without distinction of varietal type, side or batch, it was seen with the PCA correlation (>0.8) between many firmness variables and scattering at 750 and 800nm, specially when running a PCA with TDRS variables and firmness parameters alone. They were seen also some correlation (from 0.5 to 0.7) between VIS reflectance at 500 and 680nm, some firmness variables, acids and sugars.

4.3. 2nd step: k-means clustering

Once it was observed seen that there were significative correlations between TDRS parameters and fruit quality variables, the next step was the creation of "natural" fruit groups (clusters) according to their internal quality (firmness, sugars and acids). The final purpose for these new groups was to build estimation models capable of recreate the ascription of each sample to its correspondent quality group.

This methodology was used for each species, building a set of clusters for each quality attribute independently (firmness, sugars and acids). To build up these sets, the k-means clustering method was used, which produces exactly *k* different clusters of greatest possible distinction. The computer program (Statistica98, StatSoft Inc.) will start with *k* random clusters,

and then move objects (samples) between those clusters with the goal to (1) minimise variability within clusters and (2) maximise variability between clusters.

By this, the whole database of fruits was re-distributed into clusters, more homogeneous than the initial batches, when considering the single quality parameter that was used to build each set of clusters.

About the number of clusters, several trials were made with k=5 clusters, k=3 and k=2. The overall performance of the classification models was usually 10% worse when trying to discriminate between five clusters, than when classifying into three clusters, showing a logical behaviour. Finally it was considered that, form a practical approach in a future application of the technique at the industrial/grower level, three clusters seemed to be adequate, establishing in that way three quality grades for each parameter: good quality, poor and medium.

4.4. 3rd step: DA and classification models

Once the fruits have been distributed into sets of quality clusters, the next step to take was trying to estimate –to explain- those clusters using the optical TDRS information contained in the ma and m's parameters; discriminant function analysis was used for this objective.

Different models were built for each quality parameter and each fruit specie (i.e. a classification model was developed to group apples according to their firmness level, without variety distinction). To create the models, this is the classification functions, only half of the database was used. Then these models were validated using the other half of the database. Cross validations were made also combining different subsets of the database.

In the summary tables presented below (table 5a, b, c & d), scattering and absorption variables in the VIS region were used to build the models for firmness estimation, and TDRS variables in the NIR area were used as explanatory variables in all the models. The percentage of well classified samples into three quality classes for each model is shown in table 5 (A to D),

as well as the performance of the validations in brackets beside the previous one. In this table is coded also below each percentage the variable used to create the cluster for each quality attribute (extracted from the destructive tests) and on the right the number of TDRS wavelengths which conform the non-destructive estimation model.

Also, the right part of each table 5 (A to D) shows the averages of each cluster in every set of data. It can be seen that the measured ranges for the different quality attributes sampled on each fruit are wide enough to cover all the possible ripeness stages that can be found normally in market-sold fruits. Then, the models could be useful for a general purpose application of a segregating system, such us distinguishing early harvested fruits (firm, low sugar) from ripe fruits (softer, more tasty). For more precise applications, new models should be developed with an intra-varietal basis.

5. Discussion

The correlations found with this work and the models built, demonstrate that the TDRS technique presents a good potential of applicability in agricultural and food sciences to characterise internal properties of fruits and similar tissues.

For some of the fruits (tomato) tested the correlation seems to be good enough, a priori, to build continuous estimation models with low errors of estimation. In other cases (kiwi, apple, peach) the correlation is lower so the work should be focused towards classification models (non-continuous estimation).

Therefore, the initial proposal of the way to provide and select the samples has demonstrated to be efficient in screening of the TDRS methodology to estimate quality parameters, because with the acquisition of non-homogeneous, market-sold samples, high variations on quality parameters can be achieved easily. Now, to calibrate the technique and the models, in terms of validation, adjust, repeatability, etc., more controlled samples can be used to enhance the results. The final calibration of models can be done by a training process for specific sets of fruits, prior to each measurement session; an appropriate software to

recalculate the models and a systematic protocol should be developed to carry out this calibration on a "daily basis".

The estimation models include laser variables of different wavelengths, and this may complicate the device developed by obliging to incorporate a system to change the wavelength or a high number of lasers. This will cause a raise in its price, difficulties of construction and slowness when measuring a fruit. With the estimation models built at present, the possibility of using only one wavelength is not feasible because the estimation errors would be too high.

The range of wavelengths used in the firmness models (670nm, 750nm & 800nm) is in the limit of the VIS region. The first of these three corresponds to the chlorophyll spectrum peak, and the other two are in a spectral region where almost no compound presents absorbing properties. These two wavelengths may are considered "far-visible" or just the beginning of NIR, by some authors.

The classification models (sugar & acids) based on NIR TDRS variables include too many wavelengths (>5 λs) but the percentage of well classified fruits is similar than the VIS models. This may be due to the different regions where each chemical compound absorbs light along the spectrum, but it also may cause on the models an "over-learning" of the database, making more difficult future validations. More analysis should be done in reducing the number of NIR wavelengths used, taking into account also that any future development of a NIR device must be focused towards simplicity and low cost.

It has been observed that estimation models for firmness are slightly better when introducing scattering and absorption coefficients, rather than only with the first ones. This can be due to some complementary effect of absorption on the firmness information revealed mainly by the scattering. On the other hand, models with both absorption and scattering variables, at one or several wavelengths, could lack of robustness (be unstable) in future validations , due to varying relations between firmness and chemical composition. This models containing only scattering coefficients, in the case of firmness, indicates the advantage of maintaining the initial

hypothesis (light dispersion related to hardness) to gain stability, although lower segregation ability may be achieved.

The measured ranges covered for each quality attribute must be taken into account, compared with the segregation ability. With the collected database for each fruit, the ranges in quality attributes are high enough to cover most of the possible ripeness stages that every fruit could have, but these three scales (firmness, sugar and acids) were established combining samples from different varieties. When applying these classification models to one-variety samples, the segregation ability may drop down dramatically, as the corresponding scales within that variety will be much lower than the general ones. A specific study of each variety must be carried out, as well as particularised models.

The decision on the number of clusters when building the classification functions must be taken accordingly to the final use of the industrial device to be developed. For an environment with high segregational needs, five clusters may be established although the incorrectly classified samples will be more, unless better performance is achieved. For online applications, were the classification is done frequently within three quality grades (best/medium/low) or just a binary decision of pass/fail (in combination with other parameters: weight, size, defects), only three/two clusters are needed and the models developed so far are enough accurate.

Future work will be devoted to validation studies. Applicability of the developed models must be carefully analysed. System enhancements are being carried out to simplify the TDRS equipment, making it easy to use and cheaper.

6. Conclusion

TDRS has been shown to be applicable for the optical characterisation of the internal properties of fruits. The analysis of VIS and NIR data for apples, tomatoes, kiwifruits and

peaches indicates that the TDRS technique can be used to predict firmness, soluble solids content and acidity. The results support the hypothesis that the scattering coefficient should relate to texture properties, while the absorption coefficient should be associated with chemical constituents. So is shown by the certain correlation between scattering values at the far-visible region (750nm and 800nm) and several firmness variables on tomatoes, peaches and kiwis, as well as the correlation between NIR wavelengths and °Brix and acidity. More study must be performed on the relations between the physical and chemical changes caused by ripeness in the fruits, and their effect in the transmission/absorption of the TDRS light pulses. Further research is required to optimise the classification performance.

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Figure captions

Figure 1. Schematic set-up of light flux. Some of the injected photons are absorbed and some some transmitted towards deeper tissues. The photons collected by the returning fiber cross the sample along the "bannana shape area".

Figure 2. Outlining of clustering building towards model creation with DA

Table 1. All samples measured: species, varieties, number of individual fruits, experimental periods ("campaign"), visible wavelengths (VIS+farVIS) and near infrared wavelengths registered. Each wavelength originates two measurements (absorption & scattering coefficients).

Fruit	Ttl#	Variety	# fr	campaign		VIS λs (+800nm)	NIR λs (/10nm)
Apple	493	Golden Delicious	30	Nov96	Pre	650 to 750 /5nm	-
			30	Feb97	C1	675 & 800	-
			30	Feb98	C3	672, 750, & 818	900-1000
			10	Nov98	C5	-	900-1000
		Granny Smith	30	Nov96	Pre	650 to 750 /5nm	-
			15	Feb97	C1	675 & 800	-
			30	Feb98	C3	672, 750, & 818	900-1000
			10	Nov98	C5	-	900-1000
		Starking Delics.	10	Nov96	Pre	650 to 750 /5nm	-
			10	Feb97	C1	675 & 800	-
			30	Feb98	C3	672, 750, & 818	900-1000
			10	Nov98	C5	-	900-1000
		Top Red	28	Feb97	C1	675 & 800	-
		Jonagold	10	Feb97	C1	675 & 800	-
			30	Nov98	C5	672, 750, & 818	900-1000
		Cox	30	Nov98	C5	672, 750, & 818	900-1000
		Fiesta	30	Nov98	C5	672, 750, & 818	900-1000
		Gala	30	Nov98	C5	672, 750, & 818	900-1000
Kiwi	170	Hayward	90	July97	C2	675, 750 & 800	-
			80	Feb98	C3	672, 750, & 818	900-1000
Peach	200	Peach	60	July97	C2	675, 750 & 800	-
			50	July98	C4	672, 750, & 818	900-1000
		Nectarine	40	July97	C2	675, 750 & 800	-
			50	July98	C4	672, 750, & 818	900-1000
Tomato	220	Daniella type	50	July97	C2	675, 750 & 800	-
			50	July98	C4	672, 750, & 818	900-1000
		Marmande type	50	July97	C2	675, 750 & 800	-
			50	July98	C4	672, 750, & 818	900-1000
		Cherry	20	July97	C2	675, 750 & 800	-

Table 2. Tests carried out on the samples to measure firmness, colour, acidity and sugar content (standard techniques), plus the TDRS measurements (new technique). Firmness was tested in a different way on each type of fruit (penetrometry, puncture or compression).

	Destructive tests					Non-destructive	
	Standard techniques						New technique
	Magness -Taylor penetrometry	Puncture with needle	Compression with ball	Titration of acids	Refractometric index	Skin colour (VIS reflectance %)	TDRS μa & $\mu's$
Apple	*2 sides*			*2 sides*	*2 sides*	*2 sides*	*2 sides*
Peach & nectarine	*2 sides*			*2 sides*	*2 sides*	*2 sides*	*2 sides*
Kiwi		*2 sides*	*2 sides*	*2 sides*	*2 sides*	*2 sides*	*2 sides*
Tomato		*2 sides*		*2 sides x 2 depths*	*2 sides x 2 depths*	*2 sides*	*2 sides*

Table 3. Principal component analysis, including VIS %reflectance, firmness, VIS & NIR TDRS, chemical and other accessory variables. Highest relations are marked (italics). For each fruit, only the first two factors of the correspondent PCA are shown

Principal Components Analyses for each species									
		Peach		Kiwi		Apple		Tomato	
Variables		Factor 1	Factor 2	Factor 1	Factor 2	Factor 1	Factor 2	Factor 1	Factor 2
VIS reflectance %	C400	0.33	-0.17	0.37	-0.42	-0.02	*-0.73*	-0.54	0.14
	C450	*0.66*	*-0.66*	0.24	*-0.79*	-0.36	*-0.84*	*-0.88*	0.29
	C500	*0.69*	*-0.65*	0.05	*-0.95*	-0.42	*-0.85*	*-0.89*	0.20
	C550	*0.67*	*-0.63*	0.01	*-0.95*	-0.47	*-0.73*	*-0.92*	0.22
	C600	0.58	*-0.70*	0.10	*-0.96*	-0.21	*-0.94*	-0.57	0.18
	C670	0.07	*-0.87*	0.14	*-0.84*	-0.07	*-0.66*	*0.90*	0.04
TDRS absorption	MUA672	0.56	0.42	*0.80*	0.14	-0.35	0.52	-0.22	-0.11
	MUA750	0.32	0.10	0.10	0.35	*0.86*	-0.15	0.26	0.80
	MUA818	0.45	0.26	-0.52	0.10	*0.89*	-0.18	-0.21	-0.13
	MUA900	-0.08	0.49	*0.66*	0.22	*0.80*	-0.19	-0.30	0.45
	MUA950	0.42	0.35	0.56	0.16	*0.92*	-0.18	-0.17	0.47
	MUA1000	0.16	0.48	0.42	0.12	0.00	0.09	-0.02	-0.01
TDRS scattering	MUS672	0.44	*-0.62*	*0.82*	0.14	*0.81*	-0.24	0.49	0.43
	MUS750	*0.70*	-0.46	*0.86*	0.04	*0.94*	-0.07	0.41	*0.78*
	MUS818	*0.67*	-0.45	*0.61*	-0.11	*0.88*	-0.13	-0.25	-0.44
	MUS900	*0.80*	-0.22	*0.73*	0.16	*0.91*	-0.13	-0.30	0.36
	MUS950	*0.80*	-0.12	*0.74*	0.15	*0.89*	-0.15	-0.55	0.09
	MUS1000	*0.79*	-0.14	*0.71*	0.15	0.20	0.01	-0.28	0.16
Firmness (load/unl,)	F1LU	*0.70*	0.54	-	-	0.16	0.23	-	-
	SLOPE1LU	*0.73*	0.57	-	-	*0.60*	0.19	-	-
	PLAST	*-0.83*	-0.28	-	-	*0.71*	-0.14	-	-
Firmness (Mags-Tyl)	FMAXMT	*0.68*	0.55	-	-	*0.74*	0.14	-	-
	DEFORMT	*0.65*	0.58	-	-	-0.33	-0.14	-	-
	AREAMT	*0.63*	0.56	-	-	0.49	0.07	-	-
	SLOPEMT	*0.70*	0.52	-	-	*0.81*	0.19	-	-
Firmness (puncture)	PF1	-	-	*0.86*	-0.06	-	-	*-0.70*	0.32
	PT	-	-	-0.12	-0.08	-	-	-0.16	-0.22
	PA	-	-	*0.74*	-0.08	-	-	-0.47	-0.01
	PG	-	-	*0.87*	-0.03	-	-	-0.39	0.41
Acidity	ACID	-0.05	0.61	0.57	-0.01	0.31	-0.11	*-0.90*	-0.11
	ACIDInternal	-	-	-	-	-	-0.29	*-0.74*	-0.50
SSC (°Brix)	SUGAR	-0.37	0.27	0.47	0.10	0.26	-0.01	*-0.66*	0.05
	SUGARIntl	-	-	-	-	-	-0.19	-0.47	0.12
	BATCH	-0.31	0.13	-0.58	-0.04	-0.55	-0.11	-0.13	0.13
	DAY	-0.50	-0.43	0.58	0.06	*0.94*	-0.19	0.37	*0.75*
	Expl.Var	9.65	6.82	8.72	5.43	11.55	4.66	8.13	3.68
	Prp.Totl	33.29%	23.52%	31.16%	19.39%	38.48%	15.53%	28.03%	12.71%

Table 4 . Effect of the number of clusters on the classification ability. Two different DA classification models were built for each apple variety using 2 and 3 firmness clusters, respectively. The percentage of well classified individuals is usually higher when less clusters are attempted.

Apple	cox	topred	jonagold	fiesta	granny	starking	golden	gala
3 clusters	77.14	67.85	75.00	66		67.5	85.5	60
2 clusters	92.85	64.28	97.50	90	75	95	89	86

Table 5 . (part A: tomato) Summary of classification models according to fruit quality attributes for every fruit specie. Each function estimates one attribute (firmness, as puncture test slope, or max force Magness-Taylor; sugars as °Brix; or acids as meq/litre). Their performance (% of well classified fruits; bolded) is shown as well as the validation result. The right part of the table describes the characteristics of the clusters used to build the models (average value ± standard deviation).

Tomato	*Model summary*		*Clusters description (avg ± std dev)*			
Firmness with VIS	Estimating well classif. using	Puncture slope (N/mm) **81%** (val 80%) 3 λ VIS: 675, 750, 800nm	Firmness cl1: 0.5 Firmness cl2: 1.4 Firmness cl3: 2.3		N/mm ± N/mm ± N/mm ±	0.15 0.25 0.35
Sugar with NIR	Estimating well classif. using	SSC (°Brix) **98%** (val 84%) 11 λ NIR	Sugar cl1: Sugar cl2: Sugar cl3:	3.8 4.6 5.3	°Brix ± °Brix ± °Brix ±	0.31 0.21 0.25
Acid with NIR	Estimating well classif. using	Total acidity (meq/l) **98%** (val 89%) 12 λ NIR	Acid cl1: Acid cl2: Acid cl3:	25.6 43.3 55.6	meq/l ± meq/l ± meq/l ±	4.54 3.76 5.74

Table 5B. Summary of classification models for kiwi.

Kiwi	*Model summary*		*Clusters description (avg ± std dev)*			
Firmness with VIS	Estimating well classif. using	Puncture slope (N/mm) **75%** (val 75%) 3 λ VIS: 675, 750, 800nm	Firmness cl1: 1.4 Firmness cl2: 3.1 Firmness cl3: 4.4		N/mm ± N/mm ± N/mm ±	0.43 0.39 0.45
Sugar with NIR	Estimating well classif. using	SSC (°Brix) **75%** (val 62%) 8 λ NIR	Sugar cl1: Sugar cl2: Sugar cl3:	12.1 13.3 14.4	°Brix ± °Brix ± °Brix ±	0.53 0.31 0.47
Acid with NIR	Estimating well classif. using	Total acidity (meq/l) **70%** (val 66%) 10 λ NIR	Acid cl1: Acid cl2: Acid cl3:	164.1 200.1 227.3	meq/l ± meq/l ± meq/l ±	13.76 8.38 11.21

Table 5C. Summary of classification models for peach.

Peach	*Model summary*		*Clusters description (avg ± std dev)*			
Firmness with VIS	Estimating well classif. using	Fmax MgTy (N) **77%** (val 73%) 3 λ VIS: 675, 750, 800nm	Firmness cl1: 4.9 N ± 2.83 Firmness cl2: 24.2 N ± 7.29 Firmness cl3: 53.0 N ± 9.23			
Sugar with NIR	Estimating well classif. using	SSC (°Brix) **86%** (val 77%) 9 λ NIR	Sugar cl1: 10.8 °Brix ± 0.40 Sugar cl2: 12.1 °Brix ± 0.34 Sugar cl3: 13.4 °Brix ± 0.57			
Acid with NIR	Estimating well classif. using	Total acidity (meq/l) **84%** (val 75%) 10 λ NIR	Acid cl1: 90.7 meq/l ± 13.07 Acid cl2: 123.2 meq/l ± 8.46 Acid cl3: 155.6 meq/l ± 8.27			

Table 5D. Summary of classification models for apple.

Apple	*Model summary*		*Clusters description (avg ± std dev)*			
Firmness with VIS	Estimating well classif. using	Fmax MgyT (N) **76%** (val 74%) 3 λ VIS: 675, 750, 800nm	Firmness cl1: 17.5 N ± 3.11 Firmness cl2: 29.1 N ± 3.65 Firmness cl3: 41.2 N ± 4.46			
Sugar with NIR	Estimating well classif. using	SSC (°Brix) **77%** (val 71%) 5 λ NIR	Sugar cl1: 11.5 °Brix ± 1.00 Sugar cl2: 14.1 °Brix ± 0.85 Sugar cl3: 17.5 °Brix ± 1.30			
Acid with NIR	Estimating well classif. using	Total acidity (meq/l) **74%** (val 72%) 11 λ NIR	Acid cl1: 41.3 meq/l ± 10.05 Acid cl2: 70.3 meq/l ± 10.19 Acid cl3: 114.3 meq/l ± 14.80			

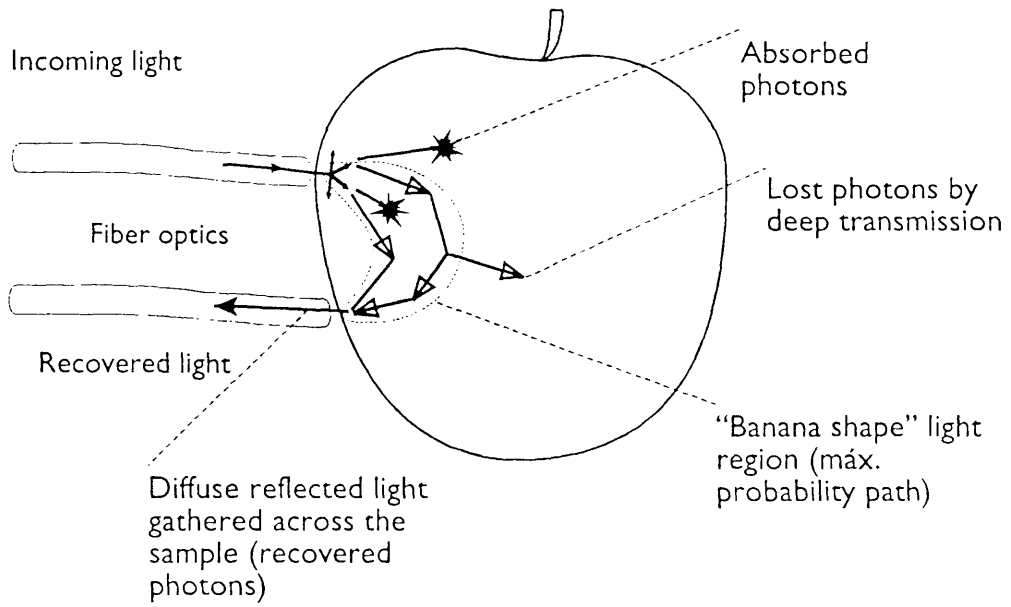

Figure 1. Schematic set-up of light flux. Some of the injected photons are absorbed and some transmitted towards deeper tissues. The photons collected by the returning fiber cross the sample along the "bannana shape area".

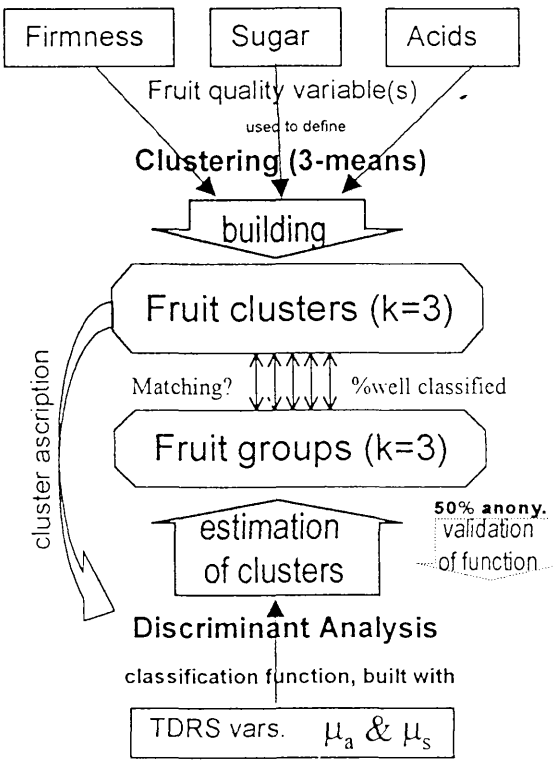

Figure 2. Outlining of clustering building towards model creation with DA