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Relating descriptive analysis and instrumental texture data of processed diced tomatoes

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Abstract

The textural properties of two varieties of tomatoes processed in duplicate by three methods (aseptic, cold-fill and hot-fill) were assessed by descriptive analysis and instrumental measurements [Kramer shear press, back extrusion and texture profile analysis (TPA)]. Sensory and instrumental data were compared and correlated using correlation analysis, principal component analysis (PCA), cluster analysis (CA) and partial least squares (PLS) regression analysis. The biplot of PLS2 with all the samples and variables explained 89% of the X variables (instrumental measurements) and 58% of the Y variables (sensory attributes). Sensory firmness was mostly explained by the instrumental firmness measurements such as the area under the curve for the Kramer and back extrusion tests. Samples were separated according to the processing method, with cold-filled samples clustered in the region where firmness variables (sensory and instrumental) were located; and hot-filled and aseptic samples grouped in the region of cohesiveness (TPA measurement), chewy (sensory) and metallic variables. These were consistent with the results from the PCA of the matrix of mean sensory texture ratings and instrumental variables across samples, run on the correlation matrix. Cluster analysis of the sensory matrix clearly classified the samples according to the processing method, whereas cluster analysis of the instrumental matrix did not. We conclude that descriptive analysis provided a more accurate account of the textural properties of diced tomatoes than the instrumental measurements we used and that PLS is the technique of choice for relating sensory and instrumental variables.

1. Introduction

In the present study, the effects of processing methods and varieties of tomatoes on the overall sensory properties of processed diced tomatoes were investigated using both sensory methodology and instrumental measurements. For sensory evaluation, a quantitative descriptive analysis method (Stone & Sidel, 1993) was used. This methodology provides quantitative descriptions of products based on the perceptions of a group of qualified subjects. For instrumental measurements, three methods were used: Kramer shear press (Kramer, Burkhardt, & Rogers, 1951), back extrusion (Kramer & Hawbecker, 1966) and texture profile analysis (Bourne, 1978; Friedman, Whitney & Szczesniak, 1963).

Sensory and instrumental measurements have been conducted and measures correlated in food products such as frozen peas (Martens, 1986), rice (Rousset, Pons & Pilandon, 1995), apples (Abbott, Watada & Massie, 1984) and pecans (Ocón, Anzaldúa-Morales, Quinters & Gastélum, 1995) among others. Although the primary objective of most textural studies is to measure sensory properties, sensory evaluation is time-consuming and costly. Therefore, many researchers choose to conduct instrumental measurements and relate those measurements to sensory evaluations. In such a case, it is crucial to extract and identify instrumental measurements that correlate best to the sensory attributes of interest. Partial least squares regression (PLS) serves that statistical purpose well. It was first used to investigate relationships between sensory and physical or chemical variables in cabbage and frozen peas by Martens (1985, 1986). PLS is a soft modeling technique used to compare two sets of data by seeking out latent variables common to both data sets (Martens & Martens, 1986).

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If several sensory variables are to be modeled based on a set of physical or chemical variables, PLS2 is used, while a separate PLS1 solution for each individual sensory variable can be used for better predictive ability.

Few studies have been devoted to correlating sensory and instrumental parameters of processed particulate tomatoes. Thus, the objectives of the present study were twofold: first, to investigate the effects of processing methods and tomato variety on diced tomatoes using both sensory and instrumental methods; and, second, to correlate and compare the sensory and instrumental measurements to identify instrumental parameters that correlated best to critical sensory variables.

2. Materials and methods

2.1. Raw materials and processing

Two common processing tomato varieties (Halley 3155 and Heinz 8892) were harvested at a 90% red maturity stage (USDA, stage 6) and processed simultaneously using one of three methods, cold-fill, hot-fill and aseptic, by the Atwater Canning Company (Atwater, CA, USA). Samples were conveyed into chlorinated water dumps, transported to steam peelers, dicers and then calcified with $CaCl_2$. Cold-filled samples were retorted in #10 cans and cooled with room temperature water. Hot-filled samples were heat treated and filled into 55 gallon drums, where they were cooled in a rotating water bath. Aseptically processed samples were heat treated, cooled and filled into laminated aseptic bags. Two processing replicates were produced for all of the tomato samples. All samples were stored at −4°C for approximately two weeks following processing. The samples in the experimental design are shown in Table 1.

Table 1
Sample identification and codes for the figures

Sample code	Processing method	Tomato variety	Process replication
As.H1.1	Aseptic	Halley	1
As.H1.2	Aseptic	Halley	2
As.Hn.1	Aseptic	Heinz	1
As.Hn.2	Aseptic	Heinz	2
Hot.H1.1	Hot-fill	Halley	1
Hot.H1.2	Hot-fill	Halley	2
Hot.Hn.1	Hot-fill	Heinz	1
Hot.Hn.2	Hot-fill	Heinz	2
Cold.H1.1	Cold-fill	Halley	1
Cold.H.1.2	Cold-fill	Halley	2
Cold.Hn.1	Cold-fill	Heinz	1
Cold.Hn.2	Cold-fill	Heinz	2

2.2. Sensory evaluation

2.2.1. Subjects

Sixteen judges (10 female (F), 6 male (M), age range 22 to 28) participated in the study. Judges were naive to sensory experiments. They were advised not to eat, drink (except for water) or smoke for at least 1 h prior to a session.

2.2.2. Sample preparation

Samples were taken out at least 5 h prior to evaluation in order to equilibrate to room temperature. Samples were served in 2 oz plastic cups (Rykoff-Sexton, Inc., Lisle, IL, USA) at room temperature. Plastic forks (Safeway Inc., Oakland, CA, USA) were provided to handle the samples. The plastic serving cups were labeled with 3-digit random codes derived with the FIZZ software (Biosystèmes, Couternon, France).

2.2.3. Design and procedures

Four 1-h sessions were devoted to term generation. The terms were generated and chosen on the basis of their uniqueness and objectivity. A scorecard was developed during these sessions and a rinsing protocol was also established. The training sessions consisted of 12 sessions, 4 group rating sessions and 8 individual booth sessions. During the term generation sessions and the training sessions, 8 commercially processed diced tomatoes (Safeway, S & W, Muir Glen, Del Monte, Millinas, Eden, Town House and Ragu) were presented. Judges were provided with standards for five attributes (dusty, sour, sweet, metallic and irritation from acid) which they had difficulties assessing. The judges were encouraged to taste each standard before each training session.

The 12 diced tomato samples were then evaluated in duplicate over 4 sessions according to a completely randomized Latin Square design, with 6 samples evaluated per session.

A 0 to 10 category scale was used to evaluate the intensity of the attributes. The FIZZ software was used to acquire the data. The definitions for all the terms were available during each session. Instructions were given on a computer monitor. Judges were instructed to taste and expectorate the samples. Two thorough rinses of drinking water (Arrowhead drinking water, Safeway, Davis, CA, USA) were taken between samples. The samples were served monadically. All the sessions were conducted under incandescent lighting in individual booths. Session length ranged from 18 to 40 min.

2.3. Instrumental evaluation

Color and texture were assessed after about 2 weeks of storage at 5°C. Samples were first equilibrated to room temperature (∼25 °C). Color was measured using a Minolta Chroma Meter (CR200, Minolta Camera Co., Ltd., Japan), recording *L*, *a* and *b* values. Three different instrumental analyses were used for texture: Kramer shear cell, back extrusion test, and the texture profile analysis (TPA) using a TA.XT2 Texture Analyzer (Texture Technologies Corp., Scarsdale, NY, USA).

For the Kramer shear test, 200 g of sample were weighed after draining over a USDA #8 screen for 1 min. Tests were run in triplicate at 1 mm/s and 90% strain using a stainless steel 5-blade probe. Firmness values were taken as the area under the curve after the maximum peak was reached and measurements were performed in triplicate.

For the back extrusion test an acrylic cylindrical cell (100 mm high, 52 mm internal diameter) was used, placing enough drained sample to fill the cell to 60 mm above the bottom of the cell (approx. 40 g). The probe traveled at a constant speed of 2 mm/s while compressing and extruding the sample down to 10 mm above the bottom of the cell (Bourne & Moyer, 1968). Firmness values were taken as the area under the curve after the maximum peak was reached. Measurements were performed in triplicate.

For the texture profile analysis test, a 1-cm^2 sample was placed on the instrument's base and compressed twice at a constant speed of 1 mm/s to 75% strain. Twenty-five replicates were taken per sample. Firmness values were obtained from the maximum peak of the first compression.

2.4. Statistical analysis

Analysis of variance (AOV) was performed on each sensory attribute with five single sources of variation (fixed effects) — judges, tomato processing method, tomato variety, batch (processing replicate), and sensory replications, and their two- and three-way interactions. Multiple means comparisons were carried out by Fisher's least significant difference at $p < 0.05$. Principal component analysis (PCA) was applied to three matrices (using the correlation matrix): the matrix of mean attribute ratings across tomato samples; the matrix of mean instrumental measurements (back extrusion, Kramer shear press and texture profile analysis); and the matrix of mean sensory texture attribute ratings and instrumental measurements combined. The matrices of mean sensory texture ratings and instrumental texture ratings were also analyzed by cluster analysis (average linkage method) to assess which set of texture measures (sensory vs. instrumental) classified the samples best in terms of processing method.

Sensory data was correlated with instrumental data by partial least squares (PLS) regression analysis, with sensory attributes as the *y* variables and instrumental measurements as the *x* variables. PLS is a soft modeling technique used to compare two sets of data by seeking out latent variables common to both data sets (Martens & Martens, 1986). If several *y*-variables are to be modeled, then a simultaneous PLS2 gives an overview, while a separate PLS1 solution for each individual Y-variable often gives better prediction ability.

AOV, PCA and cluster analyses were performed with the SAS software (SAS Institute, Inc., 1991) and PLS was performed with the Unscrambler (PLS, Computer-Aided Modeling, CAMO A/S, Norway.

3. Results and discussion

3.1. Sensory analysis

Results from the analyses of variance (AOV) of 19 sensory attribute ratings are summarized in Table 2.

Judges were a significant source of variation ($p < 0.001$) for all attributes. This is a typical descriptive analysis outcome, given that judges use different parts of the scale and may vary in their sensitivity to the attributes.

Processing methods differed significantly in 12 attributes: 3 appearance (granulated, firm-looking, and dryness of the surface), 3 taste (saltiness, sourness and metallic), 1 trigeminal (irritation from acid) and 5 textural attributes (granulated, firmness, crunchy, fibrous and chewy). However, there were no significant differences among processing methods for the aroma attributes.

The two varieties differed essentially in appearance (e.g. granulated appearance, presence of yellow veins, dryness of surface), taste (sourness) and texture (granulated and fibrous attributes).

Means and least significant differences (LSD's) for the processing methods and the varieties are presented in Tables 3 and 4, respectively. Firmness (texture) values differed significantly among processing methods, with cold-filled samples being the firmest, followed by the aseptic samples and then the hot-filled samples. This trend was observed for firm-looking, dryness of surface and crunchy attributes as well. Cold-filled samples were the most salty and irritating from acid, followed by the hot-filled and then the aseptic samples. The Heinz variety had a more granulated appearance and texture, and a drier surface, with more yellow veins than the Halley variety. Batches differed significantly for only 1 attribute — dryness of the surface, indicating that there was virtually no batch-to-batch variability. Sensory replications were significantly different for several attributes, suggesting that tomato samples were possibly changing over time. The sensory evaluation was conducted over 4 days, and although the samples were maintained in a cold room (−4°C) they may have changed somewhat over the duration of the sensory evaluation.

There were some significant 'judge by processing method' or 'judge by variety' interactions, indicative of

Table 2
Analysis of variance of 19 sensory attributes rated for diced tomato sample. *F*- ratios are shown for the sources of variations and interactions

Attributes	Judge (J)	Process (P)	Variety (V)	Batch (B)	Replication (R)	R×J	R×P	R×V	R×B	J×P	J×V	J×B	P×V	P×B	V×B
1. Granulated (App.)[a]	4.91***	10.42***	21.47***	0.19	9.91***	1.08	0.84	0.80	0.02	4.61***	0.71	1.02	1.27(NA)	0.57	1.70
2. Firm-looking (App.)	3.24***	178.07***	1.44	0.04	2.36	0.63	2.20	0.65	0.34	1.84*	0.36	0.56	1.35	3.05*	0.96
3. W/yellow veins	6.40***	0.48	10.30**	1.02	0.18	0.75	0.67	0.93	1.52	0.86	1.30	0.61	0.77	0.94	1.75
4. Dryness of surface	3.08***	46.97***	7.02**	5.63**	8.56**	0.58	0.71	0.01	0.15	2.91***	0.84	1.07	6.82**	0.52	0.44
5. Fresh tomato aroma	15.58***	2.34	0.48	0.03	3.09	2.31*	0.74	1.13	0.73	1.36	2.80**	1.00	1.31(NA)	0.97	1.37
6. Cooked tomato aroma	29.80***	1.14	0.70	0.00	7.50**	2.22*	0.23	0.80	1.25	1.61	1.21	0.44	1.25	1.05	0.20
7. Dusty (=earthy)	20.41***	2.09	0.01	0.98	0.33	2.4**	0.80	1.19	5.24*	1.93*	2.12*	0.60	0.64	0.55	0.78
8. Volatile acidity	18.72***	1.05	0.09	1.37	0.31	0.51	0.31	2.82	0.37	0.82	1.42	0.64	0.35	1.47	0.94
9. Saltiness	27.48***	202.92***	0.08	0.62	0.05	0.98	1.33	0.72	0.52	3.81***	0.69	1.15	0.06	0.36	0.72
10. Sweetness	28.66***	0.52	1.56	0.62	17.16***	3.34***	0.12	1.11	0.11	5.22***	0.53	1.96*	2.17	1.56	0.52
11. Sourness	17.66***	13.91***	0.01	0.69	8.80**	1.75	1.07	0.00	0.87	5.34***	0.68	1.15	0.20	0.01	0.60
12. Metallic	17.86***	23.05***	0.07	0.04	1.60	1.44	6.66**	4.46*	0.34	5.14***	1.32	1.26	0.39	2.47	0.00
13. Irritation acid	47.57***	68.44***	4.10*	0.82	3.15	4.36***	0.17	0.51	2.94	6.23***	1.21	1.59	0.86	2.29	0.82
14. Granulated (Tex.)[b]	6.62***	14.08***	13.24***	0.75	17.29***	3.64***	1.20	0.05	0.05	4.23***	1.39	1.35	4.25*	0.37	2.81
15. Firmness (Tex.)	13.34***	166.20***	0.36	0.22	79.68***	1.81*	8.43***	0.20	3.05	2.57***	0.85	1.15	0.38	2.66	0.16
16. Juicy	10.00***	2.80	2.78	3.78	17.35***	2.52**	0.21	0.20	0.08	2.66***	1.09	0.99	1.89	1.56	0.79
17. Crunchy	6.61***	20.29***	0.19	2.63	19.61***	1.44	1.34	1.26	0.04	2.25**	1.83*	0.74	4.82**	0.51	6.54**
18. Fibrous	9.08***	4.38**	4.68**	0.11	22.21***	1.35	0.75	0.01	0.00	3.17***	0.99	0.58	2.76	6.06**	0.19
19. Chewy	16.52***	4.91**	0.52	2.01	37.32***	1.84*	1.32	1.03	0.30	4.19***	1.47	1.08	5.27**	2.00	1.15

[a] App, appearance.
[b] Tex, texture.
*, **, *** indicates significance at $p < 0.05$, $p < 0.01$ and $p < 0.001$, respectively.

Table 3
Process method means and LSDs for all the attributes[a]

Attributes	Aseptic	Hot-fill	Cold-fill
1. Granulated	6.27a	5.50b	6.61a
2. Firm-looking	2.94a	3.16a	6.78b
3. W/yellow veins	3.84a	4.03a	3.76a
4. Dryness of the surface	5.23b	4.33a	6.55c
5. Fresh tomato	2.83a	3.24a	3.30a
6. Cooked tomato	4.75a	4.44a	4.72a
7. Dusty(=earthy)	4.74a	4.24a	4.45ab
8. Volatile acidity	3.04a	3.09a	3.38a
9. Saltiness	2.83a	2.97a	6.43b
10. Sweetness	3.14a	3.07a	2.95a
11. Sourness	4.98a	4.96a	6.06b
12. Metallic	3.64a	4.04a	2.46b
13. Irradiation from acid	3.20a	3.62a	5.45c
14. Granulated (texture)	5.55a	5.32a	6.43b
15. Firmness	5.34b	4.30a	7.68c
16. Juicy	4.62a	4.78b	5.15b
17. Crunchy	5.99a	5.84a	7.04b
18. Fibrous	6.03ab	5.57a	6.35b
19. Chewy	6.14a	5.45b	5.74ab

[a] Means with different letters are significantly different ($p < 0.05$).

Table 4
Tomato variety means and LSDs for all the attributes[a]

Attributes	Halley 3155	Heinz 8892
1. Granulated	5.66a	6.60b
2. Form-looking	4.41a	4.18a
3. W/yellow veins	3.51a	4.25b
4. Dryness of the surface	5.12a	5.62b
5. Fresh tomato	3.06a	3.19a
6. Cooked tomato	4.71a	4.56a
7. Dusty (=earthy)	4.49a	4.47a
8. Volatile acidity	3.14a	3.20a
9. Saltiness	4.05a	4.10a
10. Sweetness	2.95a	3.15a
11. Sourness	5.33a	5.34a
12. Metallic	3.41a	3.35a
13. Irritation from acid	3.92a	4.26a
14. Granulated (texture)	5.44a	6.09b
15. Firmness	5.82a	5.72a
16. Juicy	5.01a	4.69a
17. Crunchy	6.26a	6.33a
18. Fibrous	5.75a	6.22b
19. Chewy	5.71a	5.84a

[a] Means with different letters are significantly different ($p < 0.05$).

poor concept alignment among judges for some attributes.

The biplot of PC1 vs. PC2 from the PCA of the matrix of significant sensory attributes across the tomato samples is shown in Fig. 1. PC1 and PC2 explained 62.6 and 16.6% of the total variance, respectively. It can be seen that firmness (texture) was highly correlated with saltiness, irritation from acid, sourness, firm-looking and crunchy, consistent with the findings from the correlation analysis. Metallic was negatively correlated with firmness, irritation from acid, saltiness, sourness and crunchy, consistent with the correlation coefficients. Chewy was significantly correlated with fibrous and orthogonal to firmness and to the attributes that were highly correlated with firmness. It is clearly seen with this biplot that the samples were separated in terms of processing method, with cold-filled samples as firmer, saltier, crunchier, drier, more sour and granulated, and aseptic and hot-filled samples clustered together and characterized mostly by the metallic attribute.

Cluster analysis of the sensory matrix (Fig. 2) clearly separated the cold-filled samples from the hot-filled and aseptic samples.

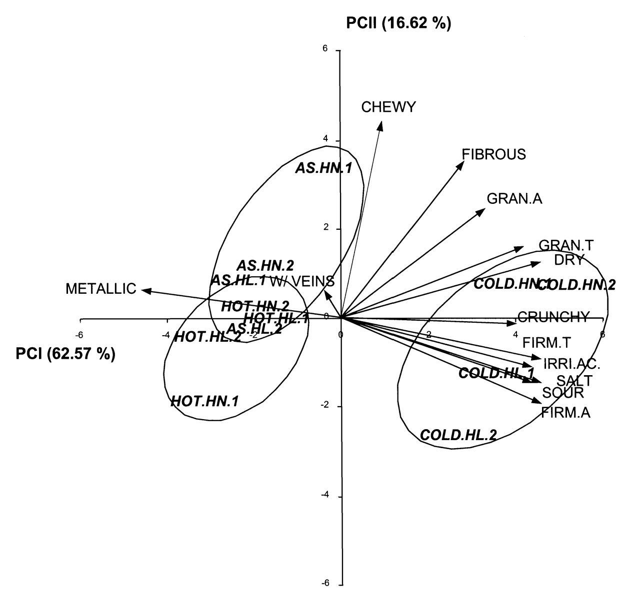

Fig. 1. PCA plot of the matrix of mean sensory attribute ratings across the samples. See Table 1 for sample key. Appearance and texture are abbreviated as A. and T., respectively. Irritation from acid is abbreviated as Irr. Ac.

3.2. Instrumental analysis

PC1 vs. PC2 of the PCA of the matrix of mean instrumental parameters across the samples is shown in Fig. 3. PC1 and PC2 accounted for 74.5 and 17.7% of the total variance, respectively. Samples were separated in terms of processing method. Cold-filled samples were characterized mostly by firmness (Kramer and back extrusion) measurements and TPA measurements. Hot-filled samples were more spread apart than cold-filled or aseptic samples and characterized mostly by TPA cohesiveness. Aseptic samples were clustered in the region opposite to TPA measurements indicating they were the least chewy, adhesive, gummy and hard in terms of instrumental parameters. It is interesting to note that the samples were also somewhat separated in terms of variety when analyzed by instrumental measurements.

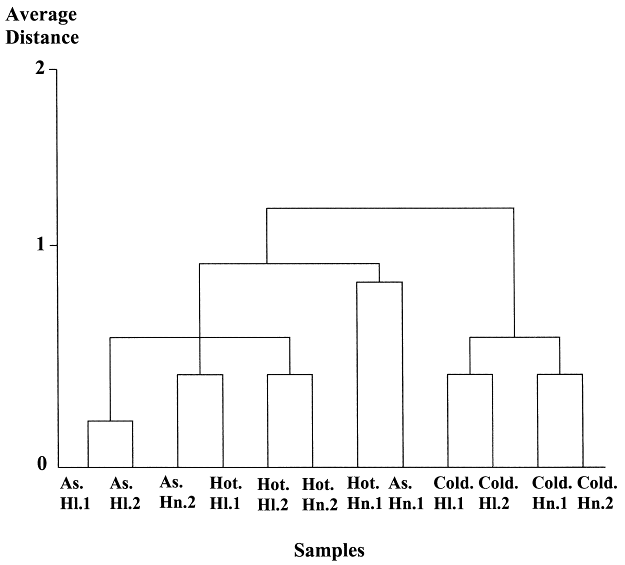

Fig. 2. Dendogram from cluster analysis (average linkage method) of 12 tomato samples by sensory textural attributes. See Table 1 for sample key.

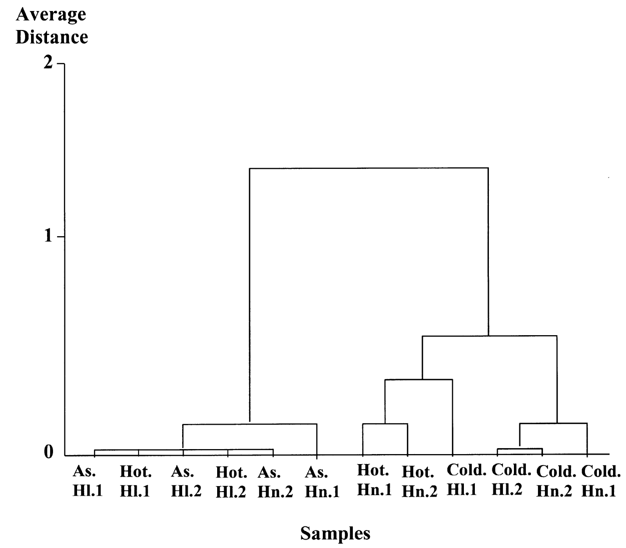

Fig. 4. Dendogram from cluster analysis (average linkage method) of 12 tomato samples by instrumental measures. See Table 1 for sample key.

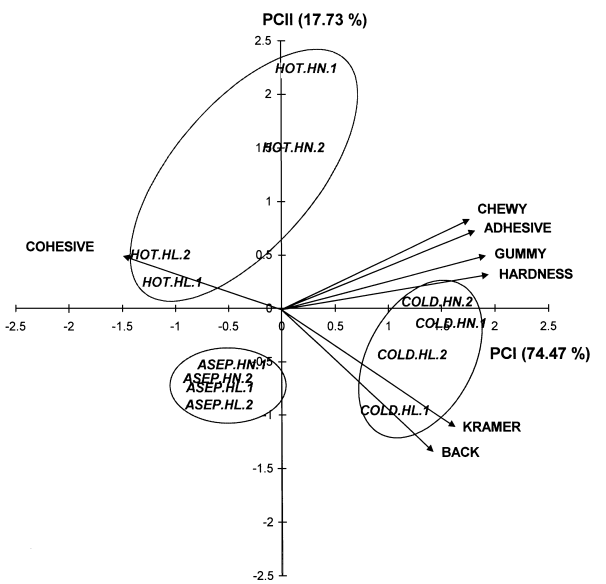

Fig. 3. PCA plot of the matrix of mean instrumental measurements across the samples. See Table 1 for sample key. 'Kramer' and 'Back' indicate Kramer firmness measurement and back extrusion firmness measurement, respectively.

Cluster analysis of the instrumental data (Fig. 4) did not separate the samples according to processing method.

3.3. Relationship between sensory attributes and instrumental parameters

The correlation matrix of the mean sensory textural ratings and instrumental parameters is shown in Table 5. Sensory firmness (texture) was correlated best with firmness measured by Kramer shear press ($r = 0.97$, $p < 0.001$) followed by firmness measured by back extrusion ($r = 0.95$, $p > 0.001$). Among the TPA parameters, hardness correlated best with sensory texture firmness ($r = 0.75$, $p < 0.01$), however to a lesser extent than the Kramer and back extrusion measurements. The sensory chewy attribute was not significantly correlated with TPA chewiness ($r = -0.38$). This may be due to the fact that sensory chewy was assessed in terms of force required to break samples into pieces whereas TPA chewiness was calculated in terms of work.

Fig. 5 shows the PCA biplot of the mean sensory textural ratings and instrumental parameters. This biplot explains 81.43% of the total variance, with PC1 and PC2 explaining 59.76 and 21.67% of the total variance, respectively. The samples were separated in terms of processing method as with the other PCA plots. Hot-filled samples were more spread apart than cold-filled or aseptic samples indicating that the hot-fill method yielded less consistent samples.

(PLS) regression analysis was performed in order to relate the 2 data sets. First, PLS2 with all the samples and all the significant sensory and instrumental variables was carried out (Fig. 6). In total, this biplot explained 89% of the instrumental measurements (x variables) and 58% of the sensory attributes (y variables). It can be seen that sensory firmness (texture) was mostly explained by instrumental firmness measurements such as the area under the curve for the Kramer and back extrusion tests, which is consistent with the findings from correlation analysis and PCA. Firmness was also explained by sensory dryness of the surface (appearance), which indicates that dry samples tended to be more firm. It is interesting to note again that

Table 5
Correlation matrix of the mean sensory textural ratings and instrumental measurements across the samples[a]

	Granulated	Firmness	Crunchy	Fibrous	Chewy	Back extrusion area	Kramer area	Hardness (TPA)	Cohesive (TPA)	Adhesive (TPA)	Gummy (TPA)	Chewy (TPA)
Granulated	1.00	–	–	–	–	–	–	–	–	–	–	–
Firmness	0.66*	1.00	–		–		–		–		–	–
Crunchy	0.66*	0.78**	1.00	–		–		–		–	–	–
Fibrous	0.70*	0.37	0.40	1.00	–		–		–		–	–
Chewy	0.35	0.06	0.22	0.74**	1.00	–		–		–		
Back extrusion area	0.73**	0.95**	0.77**	0.51	0.30	1.00	–		–		–	–
Kramer area	0.73**	0.97**	0.72**	0.54	0.21	0.97**	1.00	–		–		
Hardness (TPA)	0.58*	0.75**	0.59*	0.27	−0.27	0.60*	0.71**	1.00	–		–	–
Cohesive (TPA)	−0.26	−0.73**	−0.53	−0.11	0.11	−0.59*	−0.65*	−0.66*	1.00	–		
Adhesive (TPA)	0.48	0.56	0.45	0.13	−0.40	0.38	0.51	0.95***	−0.64*	1.00	–	–
Gummy (TPA)	0.58*	0.68*	0.51	0.26	−0.28	0.53	0.65*	0.99***	−0.59*	0.96***	1.00	
Chewy (TPA)	0.53	0.53	0.36	0.23	−0.33	0.36	0.51	0.94***	−0.48	0.94***	0.97***	1.00

[a] *, **, *** Indicate significance at $p<0.05$, $p<0.01$, $p<0.001$, respectively.

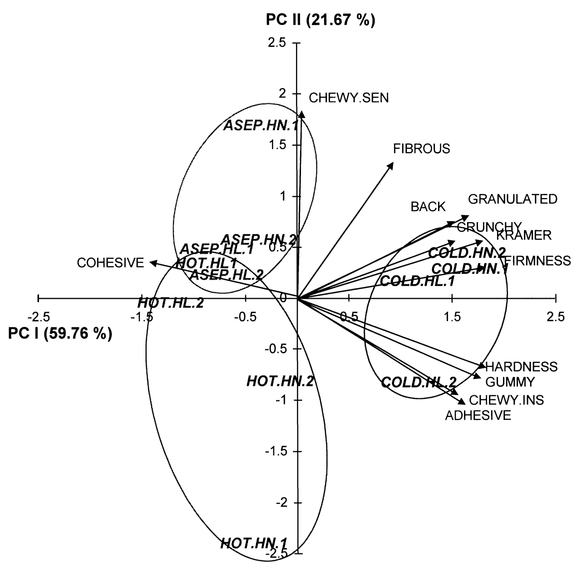

Fig. 5. PCA plot of the matrix of mean sensory texture and instrumental variables across the samples. See Table 1 for sample key. (S), (I), and (S.T.) indicate sensory attribute, instrumental measurement, and sensory texture attribute, respectively.'Kramer' and 'Back' indicate Kramer firmness measurement and back extrusion firmness measurement, respectively.

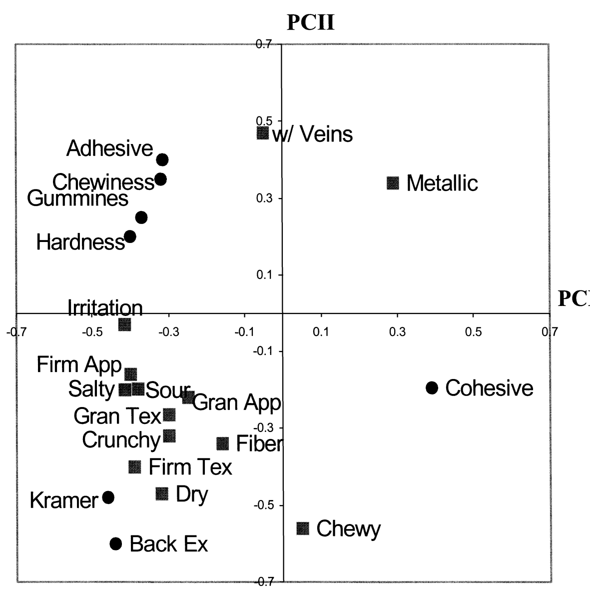

Fig. 6. PLS2 loadings for PC1 and PC2 for sensory attributes (y variable) and 7 instrumental measurements (x variables) on the 12 tomato samples. x-explained: 70%, 19%, y-explained: 47%, 11%.■,: sensory attributes;●, instrumental measurements. Appearance and texture are abbreviated as App and Tex. Granulated, irritation from acid, Kramer firmness measurement and back extrusion firmness measurement are abbreviated as Gran, Irritation, Kramer and Back Ex, respectively.

sensory chewy was not explained by instrumental chewiness, obtained by TPA measurements. In fact, it was located in the opposite side of the biplot. Most of the TPA measurements were clustered in one region of the biplot and none of them seemed to explain any of the sensory attributes. In the samples biplot, samples were separated in terms of processing methods as with all the PCA plots. Cold-filled samples were clustered in the region where firmness attributes were located and hot-filled and aseptic samples were clustered in the region where cohesive, chewy and metallic attributes were located. The hot-filled Heinz variety was characterized mostly by the 'yellow veins' (appearance) attribute. It was interesting to see that hot-filled samples were clustered by tomato variety.

PLS1 regressions were carried out to relate individual sensory attributes to the instrumental measurements. The main findings from these analyses are summarized in Table 6. The PLS1 plot with sensory firmness texture as the y variable and instrumental variables as the x variables explained 89% of the instrumental variables

Table 6
Summarized table of PLS1 plots

y-variable	x-variables	Number of components fitted	% y-explained (by PC1 and PC2)	% x-explained (by PC1 and PC2)
Sensory firmness texture	Instrumental measurements	8	80, 16	69, 20
Sensory chewy	Instrumental measurements	8	17, 7	44, 44
Sensory firm-booking	Instrumental measurements	8	81, 4	70, 18
Sensory salty	Instrumental measurements	8	85, 6	70, 17

and 96% of the sensory firmness (y variable). This biplot showed that sensory firmness was mostly explained by Kramer and back extrusion hardness measurements which corroborates the findings from PLS2. The area under the Kramer curve was the parameter that best explained firmness (sensory texture) and this confirms the findings from the correlation analysis (for Kramer, $r=0.971^{***}$, for back extrusion, $r=0.947^{***}$).

The PLS1 regression for sensory chewy as the y variable explained 88% of the instrumental variables and only 24% of the sensory chewy attribute. This indicates that chewy (sensory) was not explained well with the instrumental parameters we measured. It was anticipated that the TPA chewiness measurement would explain sensory chewy, but it did not as with the PCA plot of sensory and instrumental measurements.

The PLS1 plot for the firm-looking attribute explained 88% of the instrumental variables and 85% of the y variable. This biplot showed that sensory firm-looking attribute was best explained by instrumental firmness measurements, but not as much as sensory firmness (texture) was. It seemed as though firm-looking was located in the middle of the Kramer and TPA hardness measurements, which indicates that firm-looking is mostly explained by those two parameters.

The PLS1 biplot for saltiness was very similar to that for firm-looking, and this corresponds to the findings from the correlation analysis ($r=0.982^{***}$). This is an interesting finding because $CaCl_2$ is added to the processed diced samples to increase their firmness. In summary, sensory firmness, firm-looking (appearance) and saltiness were explained well with the instrumental parameters (PCA plot and PLS2), which indicates that instrumental measurements are mostly firmness measurements. Although TPA measurements have different terms, they seem to have similar measurements (correlation analysis) since TPA parameters were all clustered together. Also, TPA chewiness did not explain the sensory chewy attribute.

Tomato samples were separated well in terms of processing method with cold-filled samples being primarily firm, salty, dry, firm-looking; aseptic samples being chewy; and hot-filled samples being cohesive (TPA measurement).

PLS is a useful method for studying relationships between two or more tables of variables measured on a set of objects because of desirable features such as handling many x and y-variables, taking small sample sets, being realistic with respect to random noise in x and in y and multicollinearity in x and in y, giving warnings of outliers, giving estimated parameters which are easy to interpret, giving predictive validation, and giving automatic determination of optimal model complexity.

4. Conclusions

Among the three processing methods investigated in this study, the cold-fill method produced the firmest, most firm-looking and crunchiest diced tomatoes. Thus, it is concluded that this method was the least destructive of the three. Both sensory and instrumental results showed that tomato samples were grouped in terms of processing method, but not by variety. In the cluster analysis, classification of the samples according to processing method was more efficient and accurate with the sensory matrix than with the instrumental matrix (Figs. 2 and 4). We conclude that descriptive analysis provided a better assessment of the textural quality of the diced tomatoes than the instrumental measurements did.

Although not all sensory attributes were explained well with instrumental measurements in the PLS analyses (i.e. sensory chewy was not explained well with TPA chewiness), sensory textural firmness was highly correlated with instrumental parameters such as firmness measurements by Kramer shear press and back extrusion. The PLS method avoids multicollinearity problems by modeling latent variables that account for the systematic and most y-relevant ‘harmonies’ in the x-data. Thus, system analysis based on the principle of PLS offers new methods for studying relationships between two or more tables of variables measured on a set of objects.

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