Original paper

Coupled Stepwise PLS-VIP and ANN Modeling for Identifying and Ranking Aroma Components Contributing to the Palatability of Cheddar Cheese

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A consumer-oriented methodological approach for the quality evaluation of Cheddar cheese as a typical fermented food was developed. Datasets were obtained from gas chromatography/olfactometry (GC/O) analysis and sensory evaluation of 10 Cheddar cheese samples. The GC/O analysis identified 43 aroma components under the categories of 14 aroma descriptors. Consumer evaluation of palatability was performed by 59 housewives. Factor analysis of the GC/O data identified aroma descriptors that have positive or negative correlations with palatability scores. Twelve aroma components were prioritized using stepwise partial least-squares regression with variable importance in projection (PLS-VIP). An artificial neural network (ANN) model was constructed to demonstrate the nonlinear relationships among the raw GC/O data of the samples and the palatability scores. Coupling stepwise PLS-VIP and ANN resulted in successful identification and ranking of aroma components contributing to the palatability of Cheddar cheese, and in modeling their nonlinear relationships.

Keywords: partial least-squares regression-variable importance in projection (PLS-VIP), artificial neural network (ANN), gas chromatography / olfactometry (GC/O), fermented food, food kansei model

Introduction

A consumer-oriented kansei engineering approach is increasingly needed to support new product development in the food industry. Kansei engineering was founded 40 years ago and was originally developed as a methodology for transforming a consumer's feeling or image about a product into the design elements of the product (Nagamachi, 1995). Subsequently, Sagara (1994) proposed food kansei engineering, a new area of scientific and engineering research for conducting quantitative measurements of the sense of taste and food preferences by the systematization of individual techniques,

such as instrumental analyses, sensory evaluation, and multivariate analyses. The methodological combination of quantitative data and marketing tools aids in the formulation of improved strategies for product development (Akiyama *et al.*, 2012).

By applying the theoretical framework of food kansei engineering, Ikeda *et al.* (2004) proposed a food kansei model for quantitatively evaluating personal experiences of gustatory sensations during short-term eating behavior, and for utilizing the quantitative information to optimize product design and manufacturing processes. The model has been applied to investigate the relationships between instrumental and sensory data of bottled green tea beverages (Ikeda *et al.*, 2004),

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sesame-flavored dressings (Ikeda *et al.*, 2006), Danish pastries (Shibata *et al.*, 2008), prepackaged chilled espresso beverages (Michishita *et al.*, 2010), and ready-to-drink coffee beverages (Akiyama *et al.*, 2012). However, applying the model to fermented foods has remained a challenge due to their unique flavor and texture.

In general, due to their unique flavor and texture, fermented foods are often disliked by people of different cultures. Historically, processed cheeses have been more readily accepted by the Japanese compared to natural cheeses; the primary reason being that that several decades ago, the relatively tasteless flavor and texture of processed cheeses made them preferable to natural cheeses. In particular, at the time, the unique flavor and texture of natural cheeses were not well accepted among the Japanese; the annual cheese consumption per capita was less than 10 g until 1950. Decades later, overall changes in Japanese dietary habits, illustrated by the consumption of pizza, cake, and wine, were accompanied by increased consumption of natural cheeses.

In recent years, the total cheese consumption of 38 selected countries reached 1.69 million metric tons in 2012; the consumption for USA and Japan was 6,585 and 301 thousand metric tons, respectively (USDA, 2013). Despite the comparatively smaller cheese consumption of Japan, there is an increasing trend in the consumption of natural cheese products. In 2012, the total cheese consumption in Japan was 301,495 metric tons, a 6% increase over the previous year, while natural cheese consumption was 181,354 metric tons, a 12.8% increase over the previous year (MAFF, 2013). In addition, natural cheeses account of approximately 96.0% of total cheese imports in Japan, and are not only directly consumed but also utilized as ingredients of processed cheeses, mainly made from Cheddar and Gouda cheeses.

Since aroma and flavor are important factors influencing food palatability, the relationships between measured aroma components and sensory evaluation scores were also discussed based on these datasets in several previous studies (Carunchia Whetstine *et al.*, 2005; Carunchia Whetstine *et al.*, 2006) and the results of statistical analysis (Kim *et al.*, 2011; Thomsen *et al.*, 2012). In addition, there has been extensive research on the flavor of Cheddar cheese and other varieties, but despite this effort, only limited information is available on the flavor chemistry of most varieties, and none of the flavors are characterized sufficiently to permit reproduction by mixtures of pure compounds in a model cheese (Fox *et al.*, 1995; Parliament and McGorin, 2000; McGorin, 2001; Singh *et al.*, 2003).

Furthermore, many previous studies have been carried out to explore important variables from large amounts of information such as spectral data, mainly in the field of chemometrics. Factor analysis is often used, assuming the presence of potential common factors (Roy and Roy, 2009; Saurina, 2010). On the other hand, since many variables in the datasets of organic composition in food are often collinear, partial least-squares regression (PLS) is applied as a method to overcome the problem of multicollinearity and for

data reduction. Then, PLS, a linear regression method, and other nonlinear regression models are usually combined to obtain the final discriminating results (Bhandare *et al.*, 1993; Wang *et al.*, 1999; Wang *et al.*, 2003; Ciosek *et al.*, 2005). With the growing appreciation of nonlinear phenomena in general, the artificial neural network (ANN) is the most promising candidate for tractable interpretation and modeling of a large class of nonlinear problems (Borggaard and Thodberg, 1992). The ANN was employed to investigate the relationships between the principal component scores of data obtained from GC/O analysis and comprehensive palatability scores of beverage samples such as bottled green tea (Ikeda *et al.*, 2004) and prepackaged chilled espresso (Michishita *et al.*, 2010). However, in these studies, raw GC/O data of the aroma components have not been directly applied to ANN modeling. At any rate, research methods in the above-mentioned previous studies were unable to fully investigate all the relationships among the datasets obtained from instrumental analyses and consumer palatability scores, making it difficult to identify important aroma components relevant to the comprehensive palatability of natural cheeses. In this context, methodological developments are required to identify the aroma components contributing to consumer acceptance, especially the comprehensive palatability scores evaluated by consumers.

The objectives of this study were to develop a consumer-oriented methodological approach for the quality evaluation of Cheddar cheese as a typical fermented food, based on the food kansei model and the relationships between the data obtained from instrumental analyses of aroma and consumer palatability evaluations, and to identify characteristic aroma components of Cheddar cheese and the degree of these contributions to the comprehensive palatability scores evaluated by Japanese consumer panelists using coupled partial least-square regression - variable importance in projection (PLS-VIP) and ANN modeling.

Materials and Methods

Samples and aroma extraction Ten commercial Cheddar cheeses labeled as samples No.1 to 10 were selected as test samples.

Samples were commercially available (No.3, 9, and 10) and ingredients of processed cheeses (No.1, 2, 4, 5, 6, 7, and 8) (Table 1). The basic model was formulated using samples with a normal aroma and not samples with anomalous characteristics. Thus, the samples were selected from normal Cheddar cheese, indicating that samples have normal characteristics in their aroma or flavor and are normally useable for both direct consumption and as an ingredient for processed cheeses.

Aromas of the samples were analyzed using GC/MS and GC/O to identify their characteristic components and intensities. Aroma components were extracted from the samples (20 mm cubic columns) by using solvent assisted flavor evaporation (SAFE). Each sample was frozen in liquid nitrogen and then ground with an Osterizer blender (Jarden Consumer Solutions, Boca Roton, FL, USA). A 300-

Table 1. Test sample data

No.	Area of Production	Date of Manufacture	Aging period**
1	Oceania	2010.11.24	5
2	USA	2011.03.17	2
3	Japan	2011.07.20	4
4	Oceania	2010.12.10	6
5	Oceania	2011.02.07	4
6	Oceania	2012.03.05	0
7	USA	2011.11.17	-
8	Oceania	2011.01.-*	5
9	Japan	-	-
10	Europe	2012.03.27	5

*, Date was unknown, ** Unit ; month

mL aliquot of a dichloromethane solution of 3-heptanol (20 µg/mL) and 4-octanol (1.0 µg/mL) was added to the powdered sample as a standard substance, and the volatiles were extracted for 8 h using a Soxhlet apparatus (Engel *et al.*, 1999). The extract was concentrated to about 200 mL before being distilled with the SAFE apparatus. The obtained distillate was concentrated *in vacuo* by evaporation to about 1.0 mL (Onishi *et al.*, 2011).

GC/MS and GC/O analyses The concentrated extracts were analyzed with a 7890A gas chromatograph equipped with a 5975B mass spectrometer (Agilent Technologies Inc., Palo Alto, CA, USA). A DB-WAX capillary column (60 m × 0.25 mm, 0.25 µm film thickness, Agilent Technologies) was employed and the helium carrier gas flow rate was maintained at 1.6 mL/min. The oven temperature was programmed at an initial 50°C for 2 min, and was increased at 3°C/min to 220°C, and then held at the constant temperature for 75 min. The injection port was maintained at 250°C (25 psi). The extract (1.0 µL) was injected into pulsed split mode (50 psi; 60 s) to minimize thermal degradation in the injection port (Michishita *et al.*, 2010).

GC/O analysis of the concentrated extract and the dichloromethane solutions with dilution ratios of 1/3 and 1/9 were conducted using Charm Analysis™ with an Agilent 6890GC (modified by DATU, Inc., Geneva, NY, USA) (Acree *et al.*, 1984). A DB-WAX fused-silica capillary column (15 m × 0.32 mm, 0.25 µm film thickness; Agilent Technologies) was employed with a helium carrier gas flow rate of 3.2 mL/min. The oven temperature was programmed at an initial 40°C, increased at 6°C/min to 230°C, and then held at 230°C for 20 min (Michishita *et al.*, 2010). The injection port and detector were maintained at 225°C, and a 1-µL sample was injected in split-less mode. The GC effluent gas of each sample was sniffed in humidified air by a trained panelist. The odor activities of volatile components obtained by GC/O dilution analyses were represented as charm value (CV) as well as aroma descriptors (Acree *et al.*, 1984). The CV was an index of odor intensity and was calculated by integrating the time length and the dilution level as follows:

$$CV = \int_{peak} F^{n-1} di \quad \dots\dots Eq. 1$$

where F: dilution factor, n: number of dilutions, and di: length of time.

The volatile components were identified by comparing their mass spectra and Kovats indices with those of standard components. Some potent odorants found only by the GC/O analysis were tentatively identified by comparing their Kovats indices and aroma properties with those of standard components (Ikeda *et al.*, 2006; Onishi *et al.*, 2011).

Consumer evaluation of palatability Consumer evaluation of palatability was carried out by 59 consumers (housewives) in their 30s, 40s, or 50s. All panelists were housewives residing in the neighborhood where the consumer evaluation was conducted. The panelists did not receive any form of training regarding dairy products or cheeses. Female housewives were chosen as the target consumer because they were considered to have the greatest influence on daily purchases among family members in Japan regarding cheese products. Consumer panelists were selected using preliminary questionnaires on food allergy and personal preferences in regard to dairy products and cheese. The panelists gathered prior to lunch (between 10:30 am and 11:00 am), and their physical conditions and food allergies were checked before consumer evaluation. As a result, appropriate panelists were employed for consumer evaluation.

The samples were cut into 15-mm cubes, placed in plastic cups labeled with a three-digit code, and then provided to panelists. The consumer palatability tests were carried out at room temperature with fluorescent lamp lighting. The panelists tested each sample at white desks arranged in the same testing room. The panelists were allowed to carry out both finger and sniffing tests, followed by swallowing the sample. A nine-point category scale was used to evaluate consumer palatability with a hedonic rating system.

Statistical analyses Obtained datasets, including the aroma components and consumer palatability scores, were subjected to analysis of variance (ANOVA), factor analysis, correlation analysis, partial least-squares regression (PLS) and artificial neural network (ANN) modeling using JMP 9.0 (SAS Institute, Inc., Cary, NC, USA).

Factor analysis was carried out for total aroma intensity values of 14 aroma descriptors obtained by GC/O using the maximum-likelihood method and Varimax rotation for the factors in which the variance was over 1.0.

In practice, especially in process engineering, a method is required to identify the explanatory variables with the most influential on the quality of the final product. However, as mentioned earlier, many variables in the datasets of food products are often collinear. Currently, the variable importance in projection (VIP) scores obtained by PLS regression are paid increasing attention as an important measure of each explanatory variable or predictor (Chi-Hyuck *et al.*, 2009). The stepwise application of PLS-VIP was utilized in identifying the components conforming consumer palatability. Although the coefficients of determination (R^2) of PLS would decrease during the components selection

process, the order determination of specified components appeared to be more important in practical aspects. Therefore, the VIP and the weight of model (W) were monitored as threshold indicators to determine the contribution degree of each component. Thresholds for cutoff value in PLS-VIP were set as $VIP > 0.80$ and approximately $W = \pm 0.1$ according to the default setting of the software (Wold *et al.*, 1984).

ANN modeling was carried out to evaluate the link among selected aroma components and comprehensive palatability. The network had the architecture of a characteristic tri-layer perception network. This consists of one hidden layer between the input and output layers, modules of which use an error back propagation algorithm for weight to prediction error. The number of nodes in the input layer of each network was equivalent to the specified aroma components obtained from PLS-VIP. The number of hidden layers was determined by the minimum number required to improve study accuracy using four nodes. In the output layer, the number of nodes was the same as the number of equivalent palatability. The ANN model was trained with maximum iterations of 100 and number of tours of 50 times. The over-fit penalty condition was set to 0.001, and the convergence criterion was set to 0.00001. The coefficients of determination (R^2) and root mean square error (RMSE) were used to evaluate the prediction accuracy of the model.

Results and Discussion

Aroma components of Cheddar cheese GC/MS analysis identified 98 aroma components using their retention index (R_i) and density (mg/100 g) (Table 2). GC/O detected 43 aroma components (Table 3), among which, 15 aroma components corresponded to the Cheddar cheese aroma found in the literature (Singh *et al.*, 2003). Nineteen aroma components were detected by GC/O alone and not by GC/MS. The following 12 aroma components were simultaneously detected by GC/MS and GC/O: acetic acid, butyric acid, decanoic acid, diacetyl, hexanoic acid, p-cresol, phenylacetaldehyde, γ -dodecalactone, δ -decalactone, (Z)-6-dodecen-4-olide, methional and 2,5-dimethyl-4-hydroxy-3(2H)furanone. The aroma composition of sample No.4 was governed by 'potato-like' aroma (methional; 57.2% of total CVs). Similarly, sample No.5 was governed by 'sulfur' (dimethyl disulfide; 24.4% of total CVs), and No.6 by 'floral/fruity' (ethyl cinnamate; 38.2% of total CVs). From these results, samples No.4, No.5 and No.6 were discriminated from other samples by their strong character, dominated by a single aroma component (See Table 3).

Factor analysis for aroma descriptors The factor analysis for 14 aroma descriptors found six characteristic aroma factors and the cumulative percent of factors was 91.7% (Table 4). The factor loading of 'acidic/cheesy' showed the highest value (0.95) among all the aroma descriptors in factor 1. The correlation coefficients were $R = 0.85$ between 'acidic/cheesy' and 'woody,' and $R = 0.88$ between 'animal' and 'woody'. Similarly, the factor loading of

'milky' showed the highest value (0.88) among all the aroma descriptors in factor 2. The correlation coefficient was $R = 0.80$ between 'milky' and 'caramel.' Factor 3 included 'potato-like' and 'cacao-like,' and the correlation coefficient was $R = 0.90$ between 'potato-like' and 'cacao-like.' Factor 3 was considered to be governed by sample No.4 due to the considerable amounts of methional (see Table 3). In the same manner, factor 5 was governed by sample No.5 and factor 6 by sample No.6, respectively.

Figure 1 shows the positioning map of the samples by factors 1 and 2, as these factors were considered to show a common characteristic aroma of Cheddar cheese. The palatability ranking and score of factors 1 and 2 are indicated in Table 5. Sample No.9 showed the highest value of consumer palatability, followed by sample No.8. On the other hand, samples No.4, No.5, and No.6 showed lower consumer palatability values than other samples. It should be noted that the aroma composition of these samples was governed by a single aroma component as described earlier (see Table 3). The results suggested that the aroma descriptors of 'milky', 'caramel', and 'cereal' had positive correlations with consumer palatability scores, while 'acidic/cheesy', 'animal', and 'woody' had negative correlations.

Stepwise PLS-VIP identification of aroma components contributing to palatability Prior to applying PLS to the charm values (CVs) of 43 aroma components and consumer palatability scores of the samples, three samples (No.4, No.5 and No.6) were excluded from the dataset because their aroma compositions were dominated by a single aroma component as mentioned earlier (see Table 3). The remaining seven samples were applied to further modeling processes of PLS-VIP and ANN.

The first PLS trial conducted for the CVs of 43 aroma components as explanatory variables and consumer palatability scores as objective variables was successfully predicted with high accuracy ($R^2 = 0.99$). The stepwise PLS-VIP was applied to select the aroma components indicating a high contribution degree and order to palatability in the modeling. Figure 2 shows 28 aroma components selected as high contribution components in the first trial. Among all the aroma components, γ -dodecalactone (milky) showed the highest contribution to comprehensive palatability ($VIP = 2.45$). Aroma components highly contributing to the palatability scores of samples are shown in Fig. 2; thus, aroma components under the categories of 'potato-like' and 'woody' aroma were not included.

The trials were continued until all variables exceeded the selection threshold, and thus $R^2 = 0.72$ was obtained at the 9th trial (Table 6). Numbers of the explanatory variables and coefficients of determination in the PLS model decreased with increasing number of trials.

The final results of stepwise PLS-VIP are presented in Fig. 3. Four aroma components such as δ -decalactone, 1-octen-3-one, acetic acid and 2,5-dimethyl-4-hydroxy-3(2H)furanone were indicated as main aroma components of Cheddar cheese (Milo and

Table 2. Aroma components identified using GC/MS

Peak no.	Components/ Sample	No.1	No.2	No.3	No.4	No.5	No.6	No.7	No.8	No.9	No.10
1	diacetyl	5.27*	1.09	3.13	0.86	1.43	0.57	10.78	0.84	0.36	0.90
2	2-pentanone	2.09	0.82	3.72	3.80	4.53	2.66	3.22	3.28	2.08	1.29
3	valeraldehyde	1.86	0.58	1.35	1.44	2.58	0.78	0.84	1.48	0.58	5.60
4	methyl butyrate	0.49	0.30	0.85	0.52	0.62	0.60	0.64	0.24	1.27	0.95
5	3-methyl-3-buten-2-one	1.45	1.11	1.02	1.42	1.30	0.29	0.36	0.25	0.13	0.30
6	α -pinene	0.58	0.11	0.17	0.83	1.46	1.60	0.28	0.80	0.06	0.18
7	ethyl butyrate	1.67	8.87	2.34	4.39	4.09	1.82	0.89	4.20	4.34	1.76
8	hexanal	0.70	1.25	0.84	0.61	0.55	2.59	1.91	1.09	1.43	1.28
9	isobutanol	0.19	N.D.**	N.D.**	0.19	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**
10	beta-pinene	0.66	0.36	0.37	1.30	1.95	0.45	1.09	0.59	0.10	0.92
11	2-pentanol	0.12	0.06	0.14	N.D.**	0.03	N.D.**	N.D.**	0.43	N.D.**	N.D.**
12	ethyl valerate	N.D.**	0.15	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**
13	butanol	0.17	0.30	N.D.**	0.11	2.85	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**
14	myrcene	0.06	3.41	0.74	0.15	0.36	0.09	1.21	0.35	0.02	0.92
15	3-penten-2-ol	3.41	2.40	5.25	3.51	2.87	2.99	1.87	3.68	2.64	1.59
16	2-heptanone	5.87	2.74	13.90	7.65	16.10	5.44	6.20	3.21	6.62	4.30
17	methyl hexanoate	0.71	0.34	1.20	0.66	0.69	0.92	0.34	0.71	0.31	0.87
18	3-methyl-2-butenal	N.D.**	0.03	N.D.**	0.33	0.18	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**
19	limonene	3.36	4.67	5.47	3.68	4.04	8.12	48.92	17.41	1.01	43.49
20	isoamyl alcohol	N.D.**	0.21	0.48	0.34	1.21	0.08	1.13	N.D.**	0.41	9.58
21	ethyl hexanoate	2.50	8.02	1.84	2.98	2.96	0.55	0.99	4.85	1.68	0.35
22	3-methyl-3-butenol	1.95	0.49	1.22	0.83	0.47	0.52	1.29	0.84	1.71	0.94
23	amyl alcohol	1.43	0.43	0.51	1.56	1.57	1.01	0.89	1.71	0.25	4.58
24	<i>p</i> -cymene	0.14	0.11	0.09	0.15	0.43	5.51	0.90	2.00	0.08	0.79
25	acetoin	1233.00	480.02	1088.84	104.46	279.43	166.68	161.98	148.07	56.54	215.22
26	acetol	39.27	7.58	15.58	14.07	20.00	8.47	44.93	11.71	12.28	10.31
27	methyl lactate	1.26	1.58	2.76	1.34	2.21	0.94	2.13	1.00	1.54	1.87
28	2,6-dimethylpyrazine	3.28	3.20	0.33	0.53	0.14	2.32	1.13	4.61	0.79	1.40
29	ethyl lactate	0.49	6.51	0.83	0.65	1.80	0.11	2.57	1.19	2.70	0.50
30	3-hydroxy-3-methyl-2-butanone	0.57	9.41	16.54	0.20	0.87	0.38	5.87	0.37	6.30	8.51
31	hexanol	0.50	1.24	1.53	0.25	5.61	0.27	0.60	0.48	0.65	0.44
32	2-hydroxy-3-pentanone	0.65	3.96	4.85	0.29	0.85	0.25	6.11	0.51	0.75	7.17
33	2-nonanone	1.80	1.71	7.75	1.98	5.06	1.82	2.06	2.41	2.54	1.50
34	nonanal	0.30	0.42	0.28	0.15	0.13	0.31	0.38	0.54	0.43	0.57
35	trimethylpyrazine	0.49	0.77	1.03	0.05	0.04	0.17	0.18	0.33	0.16	0.21
36	ethyl octanoate	0.37	3.67	0.97	0.49	0.43	0.16	0.25	2.27	0.64	0.17
37	acetic acid	34.48	19.57	417.22	45.76	139.77	25.77	98.71	29.65	74.53	115.39
38	methional	0.32	0.82	N.D.**	1.67	0.44	N.D.**	0.09	N.D.**	0.03	0.19
39	α -copaene	N.D.**	N.D.**	N.D.**	0.01	0.05	N.D.**	N.D.**	N.D.**	N.D.**	N.D.**
40	benzaldehyde	0.43	0.35	1.25	0.77	0.17	0.30	0.62	1.17	0.24	1.22
41	tetrahydro-2-methylthiophen-3-one	N.D.**	0.31	N.D.	N.D.	N.D.	N.D.	0.13	N.D.	0.43	0.29
42	2-(methylthio)ethanol	0.21	0.07	N.D.	0.20	0.17	N.D.	0.36	N.D.	1.65	0.16
43	propionic acid	2.03	1.27	3.15	1.29	1.73	0.89	1.81	0.96	1.05	1.84
44	2,3-butanediol	8.29	2.39	1736.53	2.90	20.65	2.40	2.65	33.75	174.35	21.88
45	octanol	0.26	0.23	4.55	0.20	0.49	0.17	0.21	0.28	1.71	0.48
46	2,3-butanediol	3.31	1.89	536.14	266.89	165.03	204.47	251.25	366.88	240.47	232.41
47	dimethyl sulfoxide	0.54	3.17	N.D.	0.75	N.D.	0.12	0.05	0.08	0.29	0.02
48	2-undecanone	0.61	0.55	2.65	0.47	0.79	0.79	0.65	0.97	1.12	0.49
49	β -caryophyllene	0.05	0.11	N.D.	0.10	0.42	N.D.	N.D.	N.D.	N.D.	N.D.
50	γ -valerolactone	0.32	0.19	0.57	0.17	0.14	0.21	0.19	0.22	0.17	0.17
51	butyric acid	408.65	419.05	1338.98	584.13	703.92	394.45	412.24	449.27	535.03	616.33
52	ethyl decanoate	0.58	4.33	1.50	0.68	0.34	0.14	0.21	2.29	0.77	0.11
53	phenylacetaldehyde	1.63	2.79	6.24	2.88	0.55	1.53	3.37	4.32	0.81	3.04
54	furfuryl alcohol	0.25	0.06	0.44	0.62	0.43	0.04	0.25	0.12	0.14	0.44
55	nonanol	0.18	0.08	0.33	0.06	N.D.	0.12	0.13	0.28	0.15	0.19
56	isovaleric acid	0.68	0.74	1.69	0.46	1.23	0.23	1.07	0.63	0.19	1.16
57	methionol	0.03	0.15	N.D.	2.09	0.23	N.D.	0.06	N.D.	N.D.	5.27
58	valeric acid	5.11	6.93	16.36	5.15	5.19	4.00	5.65	8.16	6.84	6.30
59	2(5H)-furanone	0.27	0.33	0.25	0.13	0.12	0.26	0.29	0.40	0.26	0.19
60	2-acetyl-2-thiazoline	N.D.	0.04	0.03	N.D.	N.D.	0.02	N.D.	0.01	N.D.	N.D.
61	δ -hexalactone	1.93	2.28	4.94	1.41	1.09	2.22	1.26	1.76	2.04	1.15
62	2-tridecanone	0.36	0.37	1.51	0.15	0.24	0.22	0.16	0.26	0.32	0.12
63	hexanoic acid	220.15	238.34	751.24	212.21	195.83	217.27	170.26	330.72	220.36	197.91
64	benzyl alcohol	0.27	0.70	0.62	0.23	0.20	0.53	1.31	2.34	0.18	1.36
65	dimethyl sulfone	81.43	81.35	119.39	43.88	31.26	20.46	43.10	36.92	54.08	35.08
66	phenethyl alcohol	0.14	0.40	0.53	0.07	0.16	0.03	0.26	0.08	0.17	0.53
67	heptanoic acid	1.63	2.79	6.24	0.97	0.73	1.04	1.85	3.11	2.01	1.50
68	benzothiazole	0.18	0.17	0.12	0.04	0.20	N.D.	N.D.	N.D.	N.D.	N.D.
69	maltol	0.42	2.90	7.69	0.30	0.15	0.23	0.37	0.71	0.96	1.03
70	δ -octalactone	1.40	1.54	4.19	0.92	0.58	1.71	0.46	1.48	1.46	0.67
71	phenol	0.03	0.06	0.06	0.02	0.05	0.02	0.02	0.03	0.02	0.02
72	2-pentadecanone	0.21	0.22	0.71	N.D.	N.D.	0.24	0.10	0.25	0.14	0.12
73	2,5-dimethyl-4-hydroxy-3(2H)furanone	0.19	0.69	2.07	N.D.	0.09	0.09	0.06	0.08	1.79	0.10
74	ethyl myristate	0.10	1.19	0.54	0.11	0.07	0.03	0.04	0.58	0.18	0.03
75	octanoic acid	38.95	56.26	233.07	28.84	20.18	83.59	31.68	96.53	55.24	54.55
76	<i>p</i> -cresol	0.10	0.05	0.22	0.05	0.07	0.17	0.06	0.98	0.02	0.02
77	2-ethyl-4-hydroxy-5-methyl-3(2H)-furanone	0.35	0.26	2.08	N.D.	N.D.	0.12	N.D.	4.33	1.51	N.D.
78	4-hydroxy-5-methyl-2(3H)furanone	0.41	7.57	8.22	N.D.	0.76	3.80	0.25	0.47	12.62	0.51
79	γ -decalactone	0.04	0.16	0.23	N.D.	N.D.	0.05	0.11	0.08	0.12	0.02
80	nonanoic acid	1.80	2.52	5.39	0.75	0.71	1.04	0.74	2.21	1.79	0.84
81	lactic acid	N.D.	N.D.	33.27	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
82	δ -decalactone	4.11	8.43	17.27	2.65	1.32	4.22	4.24	5.42	6.57	3.09
83	(<i>E</i>)-dec-8-en-5-olide	N.D.	N.D.	N.D.	N.D.	N.D.	0.12	0.18	0.09	0.11	0.07
84	decanoic acid	26.57	32.73	153.09	12.42	6.65	45.42	13.31	55.39	31.36	27.74
85	glycerol	N.D.	0.18	1.49	N.D.	N.D.	0.11	0.22	0.31	0.17	0.18
86	δ -undecalactone	0.03	0.12	N.D.	N.D.	N.D.	0.07	0.08	30.10	0.11	0.04
87	9-decenoic acid	2.19	2.31	16.09	1.09	0.53	4.67	1.15	3.79	2.50	2.03
88	3-ethyl-4-methyl-2,5-pyrrolidinedione	0.19	0.82	0.81	0.24	N.D.	0.24	0.16	0.45	0.17	0.14
89	undecanoic acid	0.49	0.59	1.41	N.D.	N.D.	0.37	N.D.	0.35	N.D.	0.17
90	γ -dodecalactone	0.45	1.16	2.04	0.24	0.11	0.63	0.45	0.62	1.20	0.23
91	(<i>Z</i>)-6-dodecen-4-olide	N.D.	0.67	0.90	N.D.	N.D.	0.07	0.29	0.11	0.67	0.05
92	benzoic acid	26.67	37.42	84.66	19.12	13.56	13.94	13.08	30.10	18.62	21.03
93	δ -dodecalactone	1.30	1.98	5.25	0.34	0.20	1.99	1.72	2.62	2.72	1.18
94	lauric acid	6.88	6.31	26.10	2.82	1.70	6.61	1.85	6.93	4.25	12.28
95	δ -tetradecalactone	0.62	0.85	1.98	0.14	N.D.	0.53	0.27	29.06	0.39	0.21
96	myristic acid	3.11	3.67	13.13	1.05	0.81	2.91	N.D.	2.75	0.82	1.05
97	tetradecenoic acid	N.D.	N.D.	1.66	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
98	plamitic acid	7.33	8.05	18.45	3.40	1.81	N.D.	N.D.	N.D.	N.D.	N.D.
IS	3-heptanol	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00
total		2216.33	1529.29	6781.06	1413.30	1696.94	1271.80	1385.61	1773.13	1578.13	1704.02

*; Unit; mg/ 100g , Determined by the ratio of the peak area of internal standard (added 20 μ g for cheese 100g). Response factor was 1.00.

**;ND; not detected

Table 3. Potent aroma components in the samples obtained using GC/O with Charm Analysis™

Number of detection order	Descriptor	Components	Ri	Charm Value									
				No.1	No.2	No.3	No.4	No.5	No.6	No.7	No.8	No.9	No.10
12	acidic/cheesy	acetic acid	1430	18	0	131	20	103	0	83	14	27	78
20		butyric acid	1616	1264	1268	7504	1538	1921	1165	1284	1246	1562	2336
24		hexanoic acid	1840	77	98	354	73	25	81	45	106	86	50
38		decanoic acid*	2269	22	51	99	0	0	60	10	66	35	20
Total Acidic/cheesy				1381	1417	8088	1631	2049	1306	1422	1432	1710	2484
33	animal	p-cresol	2069	33	15	59	0	25	51	14	338	0	0
41		3-methylindole*	2458	154	146	2109	48	343	501	91	328	96	149
Total Animal				187	161	2168	48	368	552	105	666	96	149
2	buttery	diacetyl	1030	789	46	156	45	127	29	1477	48	22	48
Total Buttery				789	46	156	45	127	29	1477	48	22	48
1	cacao-like	2-/3-methylbutanal*	1027	21	16	0	893	244	63	344	48	42	166
Total Cacao-like				21	16	0	893	244	63	344	48	42	166
28	caramel	unknown12	1943	0	30	77	0	0	0	0	0	0	0
30		2,5-dimethyl-4-hydroxy-3(2H)furanone	2019	1084	6053	9094	28	650	533	621	865	8214	564
31, 32		2-ethyl-4-hydroxy-5-methyl-3(2H)furanone and 4-hydroxy-5-methyl-3(2H)furanone*	2051	2482	2135	5697	20	376	1104	530	10349	3949	170
36		4,5-dimethyl-3-hydroxy-2(5H)furanone*	2173	111	194	1030	40	210	200	341	675	108	180
Total Caramel				3677	8412	15898	88	1236	1837	1492	11889	12271	914
9	cereal	2-acetyl-1-pyrroline*	1326	0	0	0	0	0	0	22	0	0	7
22		2-acetyl-2-thiazoline	1732	0	259	236	0	0	159	24	57	36	0
Total Cereal				0	259	236	0	0	159	46	57	36	7
7	fatty/metallic	1-octen-3-one*	1298	59	75	38	9	11	16	153	47	41	135
15		unknown7	1495	529	422	201	145	277	359	964	1341	863	867
16		(E)-2-nonenal*	1521	534	1125	633	2041	293	693	894	1956	371	1401
18		unknown8	1600	0	29	0	0	103	0	47	0	0	41
23		2,4-(E,E)-decadienal*	1791	14	111	0	0	0	0	152	9	40	15
29		trans-4,5-epoxy-(E)-2-decenal*	1985	22	66	63	12	208	48	776	240	102	22
Total Fatty/ metallic				1158	1828	935	2207	892	1116	2986	3593	1417	2481
4	floral/fruity	unknown1	1076	0	0	0	29	0	0	0	151	18	0
21		phenylacetaldehyde	1626	16	18	27	18	12	8	17	19	6	17
25		geraniol*	1846	39	0	45	37	8	8	42	44	41	20
26		unknown10	1866	0	0	0	0	0	143	0	0	0	0
34		ethyl cinnamate *	2105	0	0	0	0	0	4038	23	0	0	0
37		o-aminoacetophenone*	2189	39	31	70	33	0	0	61	232	0	0
43		phenylacetic acid*	2548	0	11	105	27	0	0	23	84	0	0
Total Floral/ fruity				94	60	247	144	20	4197	166	530	65	37
5	green	unknown2	1104	13	23	26	7	21	13	0	0	0	18
10		unknown4	1367	0	0	0	0	0	0	0	13	0	89
17		2,4-(E,E)-octadienal*	1572	26	0	0	44	10	0	0	51	9	94
6		unknown3	1145	0	0	0	0	0	0	0	47	0	72
Total Green				39	23	26	51	31	13	0	111	9	273
13	milky	unknown6	1432	69	51	0	41	27	239	140	465	57	157
35		δ-decalactone	2160	126	242	274	42	14	150	132	174	227	44
39		γ-dodecalactone	2345	96	182	184	42	23	96	92	132	210	35
40		(Z)-6-dodecen-4-olide	2364	87	4887	6234	29	12	542	2253	566	4796	323
Total Milky				378	5362	6692	154	76	1027	2617	1337	5290	559
14	potato-like	methional	1439	356	1236	295	7110	871	240	347	55	265	395
Total Potato-like				356	1236	295	7110	871	240	347	55	265	395
3	sulfur	dimethyl disulfide*	1075	43	26	24	0	1948	0	60	0	0	14
8		2-methyl-3-furanthiol*	1311	0	0	36	0	0	0	0	0	0	0
11		unknown5	1424	13	5	0	0	18	0	0	0	0	0
19		unknown9	1605	12	14	29	0	0	0	0	0	0	0
Total Sulfur				68	45	89	0	1966	0	60	0	0	14
42	vanilla	vanillin*	2532	84	15	61	52	0	0	47	0	0	0
Total Vanilla				84	15	61	52	0	0	47	0	0	0
27	woody	unknown11	1934	0	14	46	0	0	10	0	19	14	14
44		3-phenylpropionic acid*	2608	20	24	131	0	105	13	0	26	10	0
Total Woody				20	38	177	0	105	23	0	45	24	14
Total aroma intensity				8252	18918	35068	12423	7985	10562	11109	19811	21247	7541

*; aroma component only detected by GC/O.

Table 4. Contribution ratios of 14 aroma descriptors to six characteristic aroma factors

Aroma descriptors	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6
Acidic/cheesy	0.95					
Animal	0.92					
Woody	0.84					
Milky		0.88				
Caramel		0.71				
Cereal		0.70				
Green		-0.58				
Potato-like			0.99			
Cacao-like			0.89			
Buttery				0.90		
Vanilla				0.84		
Sulfur					0.82	
Fatty/ metallic					-0.74	
Floral/ fruity						0.96
Variance	3.20	2.54	2.14	1.81	1.75	1.40
Percent (%)	22.84	18.15	15.30	12.90	12.53	9.98
Cumulative percent (%)	22.84	40.98	56.28	69.18	81.71	91.69

Table 5. Scores of factors 1 and 2 as well as palatability

Sample	Score			Order of palatability
	Factor 1	Factor 2	Palatability	
No.1	-0.14	-0.61	5.93	6
No.2	-0.66	1.59	6.24	3
No.3	2.63	0.93	6.02	4
No.4	-0.17	-0.28	5.61	8
No.5	0.05	-1.11	5.31	10
No.6	-0.28	-0.15	5.51	9
No.7	-0.84	-0.03	5.97	5
No.8	-0.06	-0.07	6.27	2
No.9	-0.84	1.25	6.39	1
No.10	0.32	-1.53	5.75	7

Reineccius, 1997; Suriyaphan *et al.*, 2001; Zehentbauer and Reineccius, 2002; Singh *et al.*, 2003). All aroma components highly contributing to the palatability of Cheddar cheese were under the following 7 categories of aroma descriptors: 'milky'; 'green'; 'fatty/metallic'; 'acidic/cheesy'; 'caramel'; 'floral/fruity'; and 'sulfur.' It was also found that descriptors such as 'milky', 'caramel', and 'floral/fruity' had positive contributions to palatability scores, while 'fatty/metallic', 'green', 'acidic/cheesy', and 'sulfur' had negative contributions. In addition, the factor scores of 'milky' and 'caramel' increased with increasing palatability scores, while 'acidic/cheesy' increased with decreasing palatability scores (see Fig. 1 and Table 6).

It should be noted that the sensory panelists in this study were all Japanese. As already mentioned, the Japanese prefer the relatively tasteless flavor and texture of processed cheeses compared to natural cheeses. These preferences are thought to be greatly influenced by the lengthy consumption of processed cheese. The results indicated the consumer preference of Japanese panelists for Cheddar cheese flavor.

Coupled modeling of PLS-VIP and ANN PLS is one of the methods used to select variables on the assumption of data linearity,

Fig. 1. Positioning map of the samples by factors 1 and 2 based on CVs of 14 aroma descriptors (●; samples having common characteristic aromas, ○; samples dominated by a single aroma component).**Table 6.** Stepwise selection of aroma components (threshold value; VIP = 0.80)

Trial time	Objective Variable	Explanatory Variable (Aroma component)	R ²	Potential factors
1th Trial		43	0.99	2
2th		28	0.99	2
3th		21	0.79	2
4th	Palatability (Sensory score)	18	0.79	2
5th		16	0.76	2
6th		15	0.72	2
7th		14	0.67	2
8th		13	0.70	2
9th		12	0.72	3

while ANN is the method used to flexibly model nonlinear relationships among the data. Aroma components highly contributing to palatability were specified by applying stepwise PLS-VIP to CVs of the GC/O data in the present study; however, the flavor of samples was not sufficiently characterized to permit its reproduction, by the mixture of pure compounds in a model cheese as mentioned earlier (Singh *et al.* 2003). This is probably due to the nonlinear relationships and mutual effects among the aroma components. Furthermore, the 'component balance theory' suggests that the Cheddar cheese flavor was produced by the correct balance and concentration of a wide range of sapid and aromatic compounds (Kosikowski and Mocquot, 1958), and thus it appeared difficult to model the Cheddar cheese aroma by simple linear modeling methods. Therefore, ANN, a nonlinear modeling method, was applied to the aroma components selected by PLS-VIP to model the relationship with comprehensive palatability scores.

The CVs of 12 aroma components identified by PLS-VIP and palatability scores were utilized as a dataset for basic ANN modeling to simulate their nonlinear relationships as well as the mutual effects contributing to palatability. The former data and the later scores were substituted into the input and output layers of

Fig. 2. Contribution degree of 28 aroma components (threshold value; VIP = 0.80)

Fig. 3. Twelve aroma components obtained by stepwise PLS-VIP analysis contributing to the palatability of Cheddar cheese (threshold value; VIP = 0.80)

Fig. 4. Typical simulation results of ANN; (a) Seven samples were used for simulation. The CVs of 2,5-dimethyl-4-hydroxy-3(2H)furanone and γ -dodecalactone were used as aroma components contributing to palatability. (b) Ten samples were used for simulation. The CVs of dimethyl disulfide and γ -dodecalactone were used as aroma components contributing to palatability. (○; local maximum value of palatability)

ANN, respectively. Because the ANN method is a relatively flexible modeling method that can be easily over-fit to the applied data set, the over-fit penalty condition was set to 0.001 and the convergence criterion to 0.00001 to avoid over-fit modeling results.

Palatability was reasonably well predicted by the ANN model, indicating high accuracy values of 0.99 and 0.97 for R^2c (calibration) and R^2v (cross validation), as well as less than 0.01 and 0.05 for RMSEc and RMSEv, respectively. Figure 4(a) showed a positive effect of 2,5-dimethyl-4-hydroxy-3(2H)furanone ('caramel') on the local maximum value of palatability to provide a searching methodology for identifying the functional aroma component. The aroma components 2,5-dimethyl-4-hydroxyl-3(2H)furanone ('caramel') and γ -dodecalactone ('milky') indicated a positive contribution to palatability by PLS-VIP, providing convincing explanations of the palatability scores using ANN modeling.

The effects of eliminated aroma components of three samples (No.4, 5, and 6) on the local maximum value of palatability were investigated by adding their CVs into the input layer of the basic model. The model showed relatively lower accuracy values of 0.95 and 0.94 for R^2c and R^2v , as well as 0.05 and 0.03 for RMSEc and RMSEv, respectively. Figure 4(b) shows that the local maximum value and its value of palatability were markedly affected only by the CV for dimethyl disulfide of sample No.5 (see Table 3). As typically shown in the curvilinear characteristic between the local maximum value and origin in Fig. 4(b), the response curved surface was found to account for both nonlinear relationships and mutual effects among aroma components, as well as palatability. The optimal aroma balance of Cheddar cheese might be designable by using a coupled PLS-VIP and ANN method to simulate the relationships among aroma intensities and consumer palatability without making numerous prototypes.

The methodology of coupled stepwise PLS-VIP and ANN modeling based on the dataset of aroma components obtained from

Fig. 5. Modified food kansei model (from Ueda *et al.*, 2008)

GC/MS as well as GC/O and sensory scores, provided a useful tool to evaluate the quality of Cheddar cheese, identifying the aroma components and their nonlinear relationships as well as mutual effects contributing to consumer palatability.

Personal attributes in the modified food kansei model affect the palatability of Cheddar cheese Figure 5 shows the modified food kansei model (Ueda *et al.*, 2008) summary of the main findings of the present study. The CVs of the aroma components were obtained by GC/O analysis as intrinsic attributes, and sensory evaluation was conducted by Japanese panelists on the basis of the perception route in the modified food kansei model. Concretely, the raw data of CVs was applied to PLS and stepwise PLS-VIP to select variables highly contributing to palatability scores. Furthermore, ANN was used to model nonlinear relationships among aroma components selected by PLS-VIP and palatability scores. In the

present study, consumer evaluation of palatability was based on the cognition route in the modified food kansei model. The results of PLS-VIP analysis suggested that personal attributes such as food culture and dietary habits might influence the comprehensive palatability scores of Cheddar cheese, as shown in the modified food kansei model. It should be noted that personal attributes in the modified food kansei model should be clarified in implementing the consumer-oriented development of food products, especially of fermented food products.

Fermented food, including cheese, has various unique flavors that depend on the production area and basic ingredients. Thus, different people show dramatically different preferences for fermented food. The effect of personal attributes, as indicated in the modified food kansei model, will present as differences in the food cognition process of fermented food, based on the dietary habits and eating experiences of consumers.

The food kansei model was developed as a method to improve the quality of food products (Ikeda *et al.*, 2004). To date, numerous studies have been performed based on this model, especially on the perception route of the model using a combination of various instrumental measurements and sensory evaluation. The modified model was proposed in consideration of personal attributes, as shown in Fig. 5 (Ueda *et al.*, 2008). In previous studies regarding food kansei engineering, the dataset was preprocessed by principal component analysis or factor analysis. Then, the processed dataset, such as principal component scores or factor scores, was used as the variables for the model construction process. This resulted in difficulty in interpreting the principal components or factors derived from the analyses. In addition, since extrinsic food attributes in the cognition route of the food kansei model are difficult to quantify, previous studies have focused on the perception route (Ikeda *et al.*, 2004; 2006; Shibata *et al.*, 2008; Michishita *et al.*, 2010). Although Akiyama *et al.* (2012) analyzed the effects of the diameter and color of straw on sensory cognition terms as a case study of the cognition route in the food kansei model, some difficulties remained in integrating the findings from the cognition route into the models constructed using the perception route data. The complexity of mutual effects among the information obtained from the routes of food perception and cognition makes it difficult to evaluate all processes.

The present study integrated the effects of personal attributes in the data analysis system as a factor in the consumer oriented product development and design method. Specifically, the main target consumers were set as Japanese housewives. Then, aroma components highly contributing to palatability scores were selected using PLS-VIP. In addition, ANN simulated the effects of aroma components on comprehensive palatability scores. A new methodology can be proposed to satisfy the preferences of specific consumers by using the data analysis procedure indicated in the present study. A further challenge is to develop a new method to merge the routes of human perception and cognition through

additional case studies based on the food kansei model.

Conclusions

The instrumentally measured data (GC/MS and GC/O) for the aroma components of Cheddar cheese were correlated with the consumer palatability scores by PLS in order to develop a quality evaluation methodology for Cheddar cheese and to determine the contribution degree of aroma components in the aroma mixture.

Based on their order in the aroma composition, the aromas of “acidic/ cheesy”, “caramel” and “fatty/ metallic” were found to be the main aroma components of Cheddar cheese. PLS was conducted to construct predictive models of consumer palatability using CVs of the aroma components. Furthermore, stepwise PLS-VIP was used to narrow down the number of specific aroma components contributing to palatability. ANN modeling was used to demonstrate the nonlinear relationships among aroma components as well as palatability. Coupling stepwise PLS-VIP and ANN resulted in successful identification and ranking of aroma components contributing to the palatability of Cheddar cheese, and in modeling their nonlinear relationships.

In the present study, Japanese consumer panelists preferred mild flavors to characteristic cheese flavors. This tendency can be understood in the context of Japan’s historical dietary culture regarding dairy products. Different people have different dietary cultures; therefore, consumer-oriented food product development requires consideration of personal attributes, shown in the modified food kansei model, especially in the case of fermented food products.

A further challenge is to perform validation tests of the model for predicting the comprehensive palatability scores of Cheddar cheese, which were evaluated by Japanese panelists in the present study. In addition, if similar experiments are performed for panelists in Euro-American nations having a long, rich dietary culture of cheese and other dairy products, entirely different results would be obtained. Focusing on personal attributes in the modified food kansei model would provide a useful cross-national perspective to compare food preferences, especially for fermented food products originating from different cultural spheres.

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