Interactions between Artificial Saliva and 20 Aroma Compounds in Water and Oil Model Systems

Saskia M. van Ruth,* Isabelle Grossmann, Mike Geary, and Conor M. Delahunty

Department of Food Science and Technology, Nutritional Sciences, University College Cork, Western Road, Cork, Ireland

The interactions between saliva components and 20 aroma compounds in water and oil model systems were systematically evaluated as a function of saliva composition and saliva/model system ratio. Air/liquid partition coefficients of dimethyl sulfide, 1-propanol, diacetyl, 2-butanone, ethyl acetate, 1-butanol, 2-pentanol, propyl acetate, 3-methyl-1-butanol, ethyl butyrate, hexanal, butyl acetate, 1-hexanol, 2-heptanone, heptanal, α-pinene, 2-octanone, octanal, 2-nonanol, and 2-decanone were determined by static headspace gas chromatography. Chain length of compounds within the homologous series determined the extent of interactions with the model system or saliva. Salts in the artificial saliva hardly interacted with aroma compounds. On the other hand, saliva proteins lowered retention of highly volatile compounds and increased retention of less volatile, hydrophobic compounds. Significant differences in volatility of compounds when artificial saliva or water was added indicated that saliva could not be sufficiently replaced by water. The model system/saliva ratio influenced air/liquid partitioning of the aroma compounds significantly for both model systems. Although saliva composition affected volatility of the aroma compounds, the saliva/model system ratio was of much greater influence.

Keywords: *Aroma; flavor; partitioning; saliva; sunflower oil; volatility*

INTRODUCTION

Flavor perception is an important factor determining consumer acceptance of food (*1*). The flavor of food is composed of a broad array of chemical compounds, which interact with olfactory receptors in the nose (odor/aroma) and with lingual receptors in the mouth (taste). During consumption, food is masticated, diluted with saliva, and warmed to 37 °C. Volatile compounds that are released during this process diffuse through the nasal cavity toward the olfactory epithelium, where the aroma is perceived (*1*). The driving force for this aroma release is the deflection from the thermodynamic equilibrium between the food phase and the air phase in the mouth (*2*).

The concentration of aroma compounds in the air phase is determined by several factors, such as the compounds' vapor pressures, solubility, concentration, partitioning in saliva, and interactions with other food constituents (*3, 4*). Control of the aroma release of food requires knowledge of the nature of interactions between aroma compounds, major food components, and saliva.

A series of interrelated partition effects determine the distribution of aroma compounds between the different phases present in the mouth. Aroma compounds distribute between the food and saliva present in the mouth, as well as between the food/saliva phase and air phase (*5*). Partitioning between the various phases occurs according to the physical properties of the aroma compounds.

Analysis of aroma compounds in the gaseous headspace above food samples has been widely used to measure partitioning between the food and the air phase, which reflects interactions in the other phases. Aroma compounds are usually present in extremely low concentrations, and in this nearly ideal state of infinite dilution, Henry's law prevails. At equilibrium, the partial pressure of the volatile in the air phase is proportional to the volatile concentration in the liquid phase. The air/liquid partition coefficient is defined as the ratio of the concentration of the aroma compound in the gas phase to its concentration in the liquid phase (*6*).

Saliva plays a prominent role in sensory perception, as its hydration/dilution of foods affects the partitioning of aroma compounds over the food, saliva, and air phase (*7*). Salivary flow rates and compositions vary widely within and among subjects (*8*). It is affected by the degree of hydration, body position, exposure to light, olfaction, smoking, (previous) stimulation, age, climatological circumstances, and circadian and circnnual rhythms (*9, 10*). The saliva/food ratio determines the extent of hydration and dilution. As a consequence, saliva volume has been reported as an important variable in theoretical models for aroma release (*11, 12*). On the other hand, saliva components such as proteins and salts can affect solubility or availability of compounds and, consequently, influence partitioning of compounds between the liquid and air phases. Despite the theoretical models, interactions of aroma compounds with saliva have not received much attention in terms of systematic experimental studies to date.

The present study examines the interactions between saliva components and 20 aroma compounds in water

* Author to whom correspondence should be addressed (telephone +353 21 4902496; fax +353 21 4270244; e-mail s.vanruth@ucc.ie).

Table 1. Retention Indices, Odor Descriptors, and Air/Liquid Partition Coefficients ($K \times 1000$) of 20 Aroma Compounds in Sunflower Oil, Whole Artificial Saliva (WSP), Artificial Saliva without Proteins (WS), and Artificial Saliva without Proteins and Salts (W) ($n = 3$)[a]

retention index	compound	odor descriptor[b]	air/liquid partition coefficient			
			oil[c]	WSP[b]	WS[ab]	W[a]
543	dimethyl sulfide	cabbage-like	14.5[d]	110.0[a]	72.5[c]	79.3[b]
560	1-propanol	alcoholic	3.8[a]	0.6[b]	0.6[b]	0.6[b]
580	diacetyl	buttery	4.9[a]	1.7[b]	1.8[b]	1.9[b]
582	2-butanone	ethereal	4.8[a]	4.6[ab]	4.4[bc]	4.3[c]
592	ethyl acetate	ethereal-fruity	5.3[c]	14.2[a]	13.4[b]	13.0[b]
635	1-butanol	fusel-like	1.3[a]	0.9[a]	0.8[a]	0.8[a]
671	2-pentanol	winey-ethereal	0.9[c]	1.7[b]	1.8[a]	1.7[b]
684	propyl acetate	fruity	2.0[c]	21.8[b]	22.8[a]	21.8[b]
713	3-methyl-1-butanol	fruity-winey	0.6[b]	1.9[a]	1.3[a]	1.2[a]
793	ethyl butyrate	fruity	1.1[c]	16.4[b]	26.4[a]	25.0[a]
799	hexanal	grassy	0.6[c]	20.8[b]	23.7[a]	23.6[a]
812	butyl acetate	ethereal-fruity	0.5[c]	20.6[b]	24.1[a]	22.8[a]
891	1-hexanol	chemical-winey	0.5[b]	2.4[b]	2.6[a]	2.4[b]
922	2-heptanone	fruity-spicy	0.5[c]	14.9[b]	16.4[a]	15.6[b]
940	heptanal	fatty-rancid	0.3[c]	29.6[b]	34.8[a]	35.8[a]
977	α-pinene	pine-like	0.3[b]	176.5[a]	176.4[a]	188.4[a]
1035	2-octanone	floral	0.3[b]	21.0[a]	22.7[a]	21.8[a]
1051	octanal	fruity	0.2[c]	33.9[b]	40.9[a]	44.1[a]
1120	2-nonanol	oily	0.3[b]	5.9[a]	6.0[a]	5.6[a]
1172	2-decanone	citrus-like	0.4[b]	27.5[a]	25.2[a]	25.5[a]
	av coefficient of variance (%)		5.4	4.0	3.5	3.6

[a] Values with different superscripts (a–c) within a row are significantly different, ANOVA and LSD tests $P < 0.05$. [b] Reference *14*.

and oil model systems as a function of saliva composition and saliva/liquid food ratio.

MATERIALS AND METHODS

Materials. Twenty aroma compounds were used in air/liquid partitioning experiments: Diacetyl, 2-butanone, ethyl acetate, 2-pentanol, hexanal, 1-hexanol, 2-heptanone, heptanal, and α-pinene were supplied by Aldrich (Steinheim, Germany). Dimethyl sulfide, ethyl butyrate, 2-octanone, and octanal were purchased from Merck (Hohenbrunn, Munich, Germany). 1-Propanol, propyl acetate, 1-butanol, butyl acetate, and 3-methyl-1-butanol were supplied by Lancaster (Walkerburn, U.K.), whereas 2-nonanol and 2-decanone were obtained from Fluka Chemie (Buchs, Switzerland).

The water and model systems were composed of distilled water and cold-pressed sunflower oil (Suma Wholefoods, Dean Clough, Hailfax, U.K.), respectively.

Three different compositions of artificial saliva were used (W, WS, and WSP). Saliva W consisted of distilled water only. Saliva WS contained the saltss NaHCO$_3$ (5.208 g), K$_2$HPO$_4$·3H$_2$0 (1.369 g), NaCl (0.877 g), KCl (0.477 g), and CaCl$_2$·2H$_2$O (0.441 g) in 1 L of water. NaN$_3$ was added at a concentration of 0.5 g/L to prevent microbial growth. The composition of WSP was identical to that of WS, but 2.160 g of mucin (porcine pancreas mucine; Aldrich) and 200000 units of α-amylase (hog pancreas α-amylase; Fluka Chemie) were added per liter of saliva.

Determination of Partition Coefficients: Static Headspace Analysis. For static headspace gas chromatography (SHGC), 2.5 mL of sample was transferred into a 10 mL headspace vial. Samples consisted of different ratios of oil/saliva and water/saliva: 0:100, 20:80, 40:60, 60:40, 80:20, and 100:0. Three types of artificial saliva were used: W, WS, and WSP. The total sample volume (water or oil model system and saliva) was maintained at a constant level throughout the experiments (2.5 mL). The aroma compounds were added to the liquid in the vial, resulting in a final concentration of 0.01% v/v per compound. The vial was closed and sealed immediately. Three replicate vials were prepared for each saliva composition and model system/saliva ratio. Samples were incubated at 37 °C and agitated at 750 rpm for 6 min in the automated headspace unit (Combipal-CTC Analytics System; JVA Analytical Ltd., Dublin, Ireland) of the gas chromatograph (Varian CP-3800; JVA Analytical Ltd.). The GC was equipped with an injector at 225 °C, a BPX5 capillary column (60 m length, 0.32

mm i.d., and 1.0 µm film thickness; SGE, Kiln Farm Milton Keynes, U.K.; helium carrier gas = 1.9 mL/min) and a flame ionization detector (FID) at 275 °C. An initial oven temperature of −30 °C was used for 1 min, followed by a rate of 100 °C/min to 40 °C. The oven temperature was maintained at 40 °C for 4 min and was subsequently programmed to 90 °C at 2 °C/min, further to 130 °C at 4 °C/min, and finally at 8 °C/min to 250 °C.

The time required to reach equilibrium between the liquid and air phase in the vial was determined in preliminary studies for both water and oil model systems. Furthermore, studies were conducted to confirm infinite dilution of the compounds at the concentration level used: lower concentrations resulted in the same partition coefficients as the concentrations used in the present study. Partition coefficients of single compounds in the oil or water model system were not significantly different from partition coefficients when 20 compounds were added simultaneously (Student's *t* test, $P < 0.05$), which demonstrates that there were no interactions between the individual aroma compounds at the concentrations used.

Four concentrations of each of the compounds were analyzed in triplicate for calibration, allowing quantification of the compounds in the air phase.

Calculation of Air/Liquid Partition Coefficients. For determination of air/liquid partition coefficients of each of the compounds, air phase concentrations (w/v) were divided by the concentrations in the liquid phase (w/v).

Statistical Analysis. Data of triplicate partition coefficient measurements for the various saliva compositions and model system/saliva ratios were subjected to univariate analysis of variance (ANOVA) to determine significant differences between the samples (*13*). Correlation between experimental and theoretical air/liquid partition coefficients was determined by calculation of Pearson's product-moment correlation coefficients (*r*). The significance level was $P < 0.05$ throughout the study.

RESULTS AND DISCUSSION

Partitioning between Air/Oil, Air/Water, and Air/Saliva. Twenty aroma compounds were added to 100% oil, saliva WSP, saliva WS, and saliva W (water). The 20 compounds are well-known aroma compounds with distinct odors (Table 1; *14*), and their selection was

Interactions between Artificial Saliva and Aroma Compounds

J. Agric. Food Chem., Vol. 49, No. 5, 2001 **2411**

based on their physicochemical properties. The headspace concentrations of the compounds in the various solutions were determined, and subsequently air/liquid partition coefficients were calculated (Table 1). Air/liquid partition coefficients indicate the affinity of the aroma compounds for the specific matrix (oil, water, or saliva). Some air/oil and air/water partition coefficients could be compared with literature values and showed similarities, for example, with air/water partition coefficients for ethyl acetate, propyl acetate, and butyl acetate published by Kieckbusch and King (*15*). The air/oil and air/water partition coefficients determined for the aldehydes hexanal, heptanal, and octanal were also in the same range as those in other studies (*16, 17*). Some slight differences between published and present data are likely to originate from the different temperatures used (25, 30, and 40 °C versus 37 °C). The homologous series of alcohols, aldehydes, ketones, and esters demonstrated a clear increase in air/water partition coefficient with increasing chain length. The number of carbon atoms was linearly related to the log transformed air/water partition coefficients of the compounds ($r = 0.912$). When compounds with the same number of C atoms were compared, generally alcohols had the lowest air/water partition coefficients, followed by ketones and subsequently esters and aldehydes. The order of the partition coefficients of the alcohol, ketone, and aldehyde groups in water is in agreement with data of Buttery et al. (*17*). For the oil model system, an inverse order was obtained for the four groups, showing that the sequence of the groups is mainly determined by the hydrophobicity of the matrix.

The air/liquid partition coefficients were significantly influenced by the type of matrix, that is, oil, WSP, WS, and W [$F(3,160) = 1023.361$, $P < 0.05$]. The oil matrix was significantly different from the three saliva matrices. Furthermore, WSP differed significantly from W, whereas WSP and WS, as well as WS and W, did not show significant differences (LSD tests, $P < 0.05$). These data show that saliva cannot be replaced by water without altering phase equilibriums. In addition, partition coefficients were significantly different for the 20 compounds [$F(19,160) = 1748.004$, $P < 0.05$]. Significant interaction between matrix (oil, water, or saliva) and compounds [$F(57,160) = 200.302$, $P < 0.05$] was observed, which indicates that the matrix affected the partition coefficient of individual compounds consistently.

Lower air/liquid partition coefficients indicate higher retention in the liquid phase. For 1-propanol, diacetyl, and 2-butanone the highest retention was observed in saliva W, which is related to the hydrophilic nature of these compounds. Their hydrophilic nature is shown by their relatively low octanol/water partition coefficients (log *P*), which are 0.25 for 1-propanol, −2.00 for diacetyl, and 0.23 for 2-butanone (*18*). Ethyl acetate and all compounds from retention index 671 onward demonstrated highest retention in oil, which is due to their generally higher molecular weight and related hydrophobic character. For most compounds no difference between WS and W was observed, whereas WSP showed for some hydrophilic compounds higher and for hydrophobic compounds lower values. The protein present in WSP is likely to bind the larger, more hydrophobic compounds and, therefore, reduce headspace concentrations. Binding of aroma compounds to proteins has been shown in various studies (*19, 20*). The present data are in agreement with previous saliva studies, which showed mucin in artificial saliva to have the largest effect on dynamic aroma release from rehydrated French beans under mouth conditions (*21*). In the latter studies, the release of, especially, aldehydes from the beans was affected by mucin. Although more compounds were affected in the present study, among them were hexanal, heptanal, and octanal, showing reductions of 12, 15, and 17%, respectively. The consistently more pronounced interactions with increasing chain length of the aldehydes are remarkable. Obviously, a larger molecule size or higher hydrophobicity results in a higher affinity for the saliva proteins.

Influence of Saliva Composition. In the second part of the study, the effect of saliva composition in combination with the model system/saliva ratio on the air/liquid partition coefficients of the 20 aroma compounds was studied. Salivas WSP, WS, and W were added to water or oil in ratios of 20:80, 40:60, 60:40, and 80:20. The partition coefficients for the water and oil model system are presented in Tables 2 and 3, respectively. The ANOVA results for the two factors saliva composition and model system/saliva ratio for the individual compounds are shown in Table 4 for both the water and oil model systems. In the water model system 12 aroma compounds were affected by the saliva composition. Dimethyl sulfide, 1-propanol, diacetyl, 2-butanone, and ethyl acetate showed increased partition coefficients when proteins were added to the saliva (WSP > WS). Contrarily, the more hydrophobic compounds, which included the aldehydes, showed a decrease in partition coefficient, and thus an increase in retention, when proteins were added.

In the oil model system, the situation was more complicated, as addition of saliva resulted in addition of a third phase. Fourteen aroma compounds were significantly affected by the saliva composition. The compounds with a low retention index, that is, dimethyl sulfide, propanol, diacetyl, 2-butanone, and ethyl acetate, showed a "salting-out" effect by addition of proteins to the saliva, which corresponds to phenomena observed in the water model system. These more hydrophilic compounds will be distributed over the oil and saliva phases, with a considerable proportion in the water phase. Consequently, the effect of the saliva composition is rather similar to the one water phase model system. Some larger, more hydrophobic compounds showed also significant differences in partition coefficients between the saliva compositions, but these differences were not consistent.

Influence of Model System/Saliva Ratio. The model system/saliva ratio had a limited effect on the compounds in the water system. The partition coefficients of only eight relatively volatile compounds were significantly affected. These compounds demonstrated an increased salting out effect with higher saliva ratios. This effect is related to the concentration of salts and proteins, as addition of saliva maintained the one phase system. Data confirm saliva composition effects described in the previous section.

In the oil model system, all compounds but 1-butanol were significantly influenced by the model system/saliva ratio. 1-Propanol and diacetyl showed largest retention in systems with a high saliva ratio. All other compounds were more retained in the systems with a high oil ratio. This effect is due to the different solubilities and affinities of the compounds for the oil and saliva phase.

2412 *J. Agric. Food Chem.,* Vol. 49, No. 5, 2001

van Ruth et al.

Table 2. Air/Liquid Partition Coefficients ($K \times 1000$) of 20 Aroma Compounds in Water with Addition of Whole Artificial Saliva (WSP) and Artificial Saliva without Proteins (WS) in Various Water/Saliva Ratios (20:80, 40:60, 60:40, and 80:20 v/v) ($n = 3$)

compound	WSP				WS			
	20:80	40:60	60:40	80:20	20:80	40:60	60:40	80:20
dimethyl sulfide	87.2	86.8	84.7	80.5	69.9	67.2	64.6	62.1
1-propanol	0.6	0.6	0.6	0.6	0.6	0.6	0.5	0.5
diacetyl	1.7	1.6	1.6	1.5	1.7	1.5	1.2	1.3
2-butanone	4.4	4.5	4.5	4.3	4.3	4.3	4.1	4.1
ethyl acetate	13.4	13.7	13.5	13.1	13.2	13.0	12.3	12.3
1-butanol	0.8	0.9	0.9	0.8	0.8	0.8	0.8	0.8
2-pentanol	1.7	1.8	1.8	1.7	1.8	1.8	1.7	1.7
propyl acetate	21.8	22.3	22.0	21.5	22.5	22.1	21.0	20.9
3-methyl-1-butanol	1.2	1.3	1.3	1.3	1.3	1.4	1.2	1.3
ethyl butyrate	22.0	19.9	20.0	21.0	25.8	25.2	24.6	23.6
hexanal	21.9	21.6	21.8	22.2	23.4	23.0	22.4	21.8
butyl acetate	22.0	21.8	21.6	21.3	23.6	22.9	22.3	21.5
1-hexanol	2.3	2.4	2.4	2.4	2.6	2.6	2.6	2.5
2-heptanone	15.6	15.9	15.8	15.3	16.1	15.7	15.4	14.9
heptanal	32.4	31.0	31.6	32.4	34.0	33.3	34.1	31.5
α-pinene	183.7	178.4	187.8	168.4	155.2	138.3	179.6	109.5
2-octanone	21.5	22.1	21.8	21.3	22.1	21.5	21.7	20.5
octanal	37.2	34.3	35.5	37.1	40.0	39.3	42.4	37.8
2-nonanol	5.7	6.0	6.0	6.1	6.0	6.0	6.0	6.2
2-decanone	25.8	26.7	26.5	27.6	26.2	26.2	26.9	28.9
av coefficient of variance (%)	4.1	3.1	2.2	4.0	4.4	4.3	1.2	6.6

Table 3. Air/Liquid Partition Coefficients ($K \times 1000$) of 20 Aroma Compounds in Sunflower Oil with Addition of Whole Artificial Saliva (WSP), Artificial Saliva without Proteins (WS), and Artificial Saliva without Proteins and Salts (W) in Various Oil/Saliva Ratios (20:80, 40:60, 60:40, and 80:20 v/v) ($n = 3$)

compound	WSP				WS				W			
	20:80	40:60	60:40	80:20	20:80	40:60	60:40	80:20	20:80	40:60	60:40	80:20
dimethyl sulfide	52.5	37.1	22.3	17.1	27.6	16.4	9.6	7.7	41.0	23.1	17.0	13.7
1-propanol	0.9	0.9	1.2	1.7	0.6	0.9	1.1	1.6	0.7	0.8	1.0	1.6
diacetyl	1.8	2.2	2.4	2.9	1.8	1.9	1.8	2.1	2.2	2.4	2.6	3.4
2-butanone	4.8	5.0	4.6	4.5	4.1	4.0	3.5	3.4	4.3	4.0	3.9	4.1
ethyl acetate	10.9	9.4	6.8	5.8	9.4	7.1	4.9	4.2	9.7	7.0	5.8	5.2
1-butanol	0.9	0.9	0.9	0.9	0.8	0.9	0.8	0.9	0.8	0.7	0.8	0.9
2-pentanol	1.3	1.1	0.9	0.8	1.4	1.2	0.8	0.7	1.3	0.9	0.8	0.8
propyl acetate	7.8	5.2	3.0	2.3	7.6	4.2	2.3	1.8	7.3	3.7	2.7	2.1
3-methyl-1-butanol	1.0	0.8	0.6	0.5	1.1	0.8	0.5	0.5	1.0	0.7	0.6	0.5
ethyl butyrate	3.1	2.2	1.4	1.2	3.4	2.0	1.2	1.1	3.4	1.7	1.3	1.2
hexanal	3.1	1.7	0.9	0.7	2.8	1.3	0.7	0.5	2.8	1.2	0.9	0.7
butyl acetate	2.8	1.6	0.9	0.6	2.8	1.3	0.6	0.5	2.6	1.1	0.7	0.6
1-hexanol	0.8	0.6	0.6	0.5	1.1	0.7	0.6	0.5	1.0	0.6	0.6	0.5
2-heptanone	1.8	1.0	0.7	0.5	1.7	0.9	0.5	0.5	1.6	0.7	0.6	0.5
heptanal	1.6	0.8	0.5	0.3	1.3	0.6	0.4	0.3	1.4	0.6	0.4	0.3
α-pinene	2.6	1.2	0.6	0.4	1.7	0.7	0.4	0.3	1.8	0.7	0.5	0.4
2-octanone	1.0	0.5	0.4	0.3	0.8	0.5	0.4	0.3	0.8	0.4	0.4	0.3
octanal	1.0	0.5	0.3	0.3	0.7	0.4	0.3	0.2	0.6	0.3	0.3	0.2
2-nonanol	0.5	0.3	0.3	0.3	0.5	0.4	0.3	0.3	0.4	0.3	0.3	0.3
2-decanone	0.8	0.5	0.4	0.4	0.7	0.5	0.4	0.4	0.5	0.4	0.4	0.4
av coefficient of variance (%)	25.4	9.7	9.2	5.1	13.1	12.8	13.7	14.0	20.1	13.9	12.3	6.0

The experimental partition coefficients for the different model system/saliva ratios as presented in Tables 2 and 3 were compared with theoretical partition coefficients. These theoretical partition coefficients were based on the measured air/100% oil, air/100% water, and air/100% saliva partition coefficients. The theoretical air/liquid partition coefficients were calculated according to the equations for determining partition coefficients (K) in three-phase systems (eq 1) developed by Buttery et al. (*22*). K is the ratio of the solute concentration in the air to the solute concentration in the liquid phase, K_w is the air/water partition coefficient, K_0 is the air/oil partition coefficient, and F_w and F_o are the volumetric fractions of water and oil in the liquid phase, respectively. The air/liquid partition coefficient was calculated as follows:

$$K = 1/[(F_w/K_w) + (F_o/K_o)] \quad (1)$$

Experimental partition coefficients correlated very well with the theoretical partition coefficients. Correlation coefficients of $r = 0.996$, 0.975, and 0.993 were determined for oil combined with WSP, WS, and W, respectively. This resulted in a high correlation coefficient for the oil model system overall ($r = 0.966$). A similar correlation was found for the water model system ($r = 0.986$), with correlation coefficients for water and WSP and WS of 0.997 and 0.980, respectively. Despite the high correlation coefficients, experimental values were consistently lower for both model systems, that is, 7.4% for water and 15.8% for the oil model system. It might be possible that a more or less emulsified system was formed during incubation (agitation = 750 rpm). The interface might have retained compounds, which in turn lowered concentrations in the headspace.

Conclusions. Both saliva composition and saliva/ model system ratio affected the volatility of 20 aroma

Interactions between Artificial Saliva and Aroma Compounds

J. Agric. Food Chem., Vol. 49, No. 5, 2001 **2413**

Table 4. Analysis of Variance Results: Probability Levels (Percent) Associated with *F* Values of the Two Factors Saliva Composition and Model System/Saliva Ratio for the Air/Liquid Partition Coefficients of 20 Aroma Compounds in Water and Oil Model Systems[a]

	water		oil	
	saliva composition	saliva ratio	saliva composition	saliva ratio
dimethyl sulfide	**0.0**	**0.0**	**0.0**	**0.0**
1-propanol	**0.0**	**0.1**	**0.0**	**0.0**
diacetyl	**0.0**	**0.0**	**0.0**	**0.0**
2-butanone	**0.0**	**0.0**	**0.0**	**0.0**
ethyl acetate	**0.0**	**0.0**	**0.0**	**0.0**
1-butanol	38.4	38.9	47.3	43.2
2-pentanol	17.9	**0.7**	35.5	**0.0**
propyl acetate	37.7	**0.1**	**0.5**	**0.0**
3-methyl-1-butanol	**0.3**	5.9	27.4	**0.0**
ethyl butyrate	**0.0**	**0.9**	**0.0**	**0.0**
hexanal	**0.3**	29.2	**1.7**	**0.0**
butyl acetate	**0.1**	7.7	**0.3**	**0.0**
1-hexanol	**0.0**	73.9	**0.4**	**0.0**
2-heptanone	69.1	7.1	6.0	**0.0**
heptanal	5.5	31.6	**0.0**	**0.0**
α-pinene	**1.8**	41.6	39.1	**0.0**
2-octanone	81.6	29.6	**3.1**	**0.0**
octanal	**0.5**	8.6	**0.0**	**0.0**
2-nonanol	15.0	5.6	**2.8**	**0.0**
2-decanone	59.7	5.1	5.7	**0.0**

[a] In bold: significant probabilities at a 5% level.

compounds. Saliva composition affected air/liquid partition coefficients of aroma compounds in both the water and oil model systems, showing a salting out effect for hydrophilic compounds and binding of hydrophobic compounds by proteins present in saliva. The significant differences between water and saliva lead to the conclusion that water does not replace saliva sufficiently. The ratio of saliva to model system is of great influence on the partitioning of aroma compounds. When the present data are related to aroma release in the mouth, liquid food/saliva ratios seem to influence partitioning of aroma compounds between liquid food and air phase more and are, therefore, of greater importance than the composition of the saliva.

LITERATURE CITED

(1) Plug, H.; Haring, P. The role of ingredient-flavour interactions in the development of fat-free foods. *Trends Food Sci. Technol.* **1993**, *41*, 150−152.

(2) Overbosch, P.; Achterof, W. G. M.; Haring, P. G. M. Flavor release in the mouth. *Food Rev. Int.* **1991**, *7*, 137−184.

(3) Landy, P.; Courthaudon, J.-L.; Dubois, C.; Voilley, A. Effect of interface in model food emulsions on the volatility of aroma compounds. *J. Agric. Food Chem.* **1996**, *44*, 526−530.

(4) Kinsella, J. E. Flavor perception and binding. *Int. News Fats, Oils Relat. Mater.* **1990**, *1*, 215−226.

(5) Solms, J.; Osman-Ismail, F.; Beyeler, M. The interaction of volatiles with food components. *Can. Inst. Food Sci. Technol. J.* **1973**, *6*, A10−A16.

(6) Taylor, A. J. Physical chemistry of flavour. *Int. J. Food Sci. Technol.* **1998**, *33*, 53−62.

(7) Taylor, A. J. Volatile flavor release from foods during eating. *Crit. Rev. Food Sci. Nutr.* **1996**, *36*, 765−784.

(8) Pangborn, R. M.; Lundgren, B. Salivary secretion in response to mastication of crisp bread. *J. Texture Stud.* **1978**, *8*, 463−472.

(9) Wisniewski, L.; Epstein, L. H.; Caggiula, A. R. Effect of food change on consumption, hedonics, and salivation. *Physiol. Behav.* **1992**, *52*, 21−26.

(10) Dawes, C. Physiological factors affecting salivary flow rate, oral sugar clearance, and the sensation of dry mouth in man. *J. Dent. Res.* **1987**, *66*, 648−653.

(11) Harrison, M. Effect of breathing and saliva-flow on flavour release from liquid foods. *J. Agric. Food Chem.* **1998**, *46*, 2727−2735.

(12) de Roos, K. B.; Wolswinkel, K. Non-equilibrium partition model for predicting flavour release in the mouth. In *Trends in Flavour Research*; Maarse, H., van der Heij, D. G., Eds.; Elsevier: Amsterdam, The Netherlands, 1994; pp 53−57.

(13) O'Mahony, M. *Sensory Evaluation of Food*; Dekker: New York, 1986.

(14) Arctander, S. *Perfume and Flavor Chemicals*; Allured Publishing: Carol Stream, IL, 1994.

(15) Kieckbusch, T. G.; King, C. J. Partition coefficient for acetates in food systems. *J. Agric. Food Chem.* **1979**, *27*, 4−507.

(16) Hall, G.; Andersson, J. Volatile fat oxidation products. II. Influence of temperature on volatility of saturated mono- and di-unsaturated aldehydes in liquid media. *Lebensm. Wiss. Technol.* **1983**, *16*, 362−366.

(17) Buttery, R. G.; Ling, L. C.; Guadagni, D. G. Volatilities of aldehydes, ketones, and esters in dilute water solution. *J. Agric. Food Chem.* **1969**, *17*, 385−389.

(18) Lide, D. R. *CRC Handbook of Chemistry and Physics*; CRC Press: New York, 1997.

(19) Le Thanh, M.; Thibeaudeau, P.; Thibaut, M. A.; Voilley, A. Interactions between volatile and non-volatile compounds in the presence of water. *Food Chem.* **1992**, *43*, 129−135.

(20) O'Keefe, S. F.; Wilson, L. A.; Resurreccion, A. P.; Murphy, P. A. Determination of the binding of hexanal to soy glycinin and β-conglycinin in an aqueous model system using a headspace technique. *J. Agric. Food Chem.* **1991**, *39*, 1022−1028.

(21) van Ruth, S. M.; Roozen, J. P.; Nahon, D. F.; Cozijnsen, J. L.; Posthumus, M. A. Flavour release from rehydrated French beans (*Phaseolus vulgaris*) influenced by composition and volume of artificial saliva. *Z. Lebensm. Unters. Forsch.* **1996**, *203*, 1−6.

(22) Buttery, R. G.; Guadagni, D. G.; Ling, L. C. Flavor compounds volatilities in vegetable oil and oil−water mixtures: estimation of odor thresholds. *J. Agric. Food Chem.* **1973**, *21*, 198−201.