

Behavior of Flavor Compounds in Model Food Systems: a Thermodynamic Study

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Physicochemical parameters, such as hydrophobicity, water solubility, and volatility, of four flavor compounds (ethyl acetate, ethyl butyrate, ethyl hexanoate, and 2-pentanone) were determined. The amount of flavor compounds released from different model matrices (mineral water, purified triolein, an oil-in-water emulsion, a carbohydrate matrix, and a complex matrix containing lipids and carbohydrates) into the gaseous phase was determined at thermodynamic equilibrium, at 37 °C, by static headspace gas chromatography. The degree of interaction between the flavor compounds and the matrix components was shown by measuring the percentage retention using the water matrix as the reference. The partition of flavor compounds was principally dependent on their hydrophobicity. Physicochemical interactions that occurred in the different media led to different degrees of flavor retention. An impact of fat on flavor retention was demonstrated when a water matrix and an oil-in-water matrix or carbohydrate and complex matrices were compared. A carbohydrate impact on flavor compound retention was also detected, which was evident even in the presence of lipids.

KEYWORDS: Flavor compounds; volatility; partitioning; headspace gas chromatography; triolein; carbohydrates

INTRODUCTION

Foods are a mixture of volatile and nonvolatile components. Flavor compounds can be naturally present in foods or can be added to balance, for example, the losses or degradations that may occur during the fabrication process. Aromatization is a key step in the production of foods and is an important part of the sensory properties, which are at the center of consumer preferences.

The key features influencing transfer and release of flavor compounds are their chemical nature and the composition and the structure of foods. Food matrices are generally multiphase, containing liquid, solid, and gaseous phases. As a function of their affinity for the different phases, flavor compounds partition between phases, and this repartition can change the perceived flavor during eating. Flavor partition depends on the affinity of the compounds for the different phases (aqueous, lipidic, etc.) and on their availability for release into the gaseous phase.

In the literature there are a lot of studies showing flavor compound behavior with food components using simple matrices. However, studies with complex matrices or real foods are more complicated, and fewer have been reported (1–4). The nature of the different components such as proteins, fats, or carbohydrates has a great impact on flavor compound retention (5–11). Physicochemical interactions can modify migration of flavor compounds, thus enhancing or decreasing flavor release. Partitioning between the various phases occurs according to the physical properties of the flavor compounds. Flavor compound concentration in the gaseous phase above the matrix is often used to measure the degree of partitioning between the matrix and the gaseous phase, and this indicates the level of interaction between the flavors and the matrix. This partition coefficient therefore defines the *maximum potential extent* of the flavor release. Lipids are the food ingredients that have been shown to have the most effect on the partitioning of flavor compounds between product and gaseous phase (8).

Carbohydrates can also lead to a retention of flavor compounds in the matrix, this reduction in volatility being due to interactions that can occur between carbohydrates such as starches and flavor compounds (12, 13). Carbohydrates such as pectins can also play a role in retention due to their thickening effect (10, 14, 15).

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
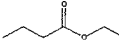
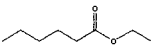

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Table 1. Flavor Compounds and Their Molecular Weights (M_w), Densities (d), Boiling Points (bp), and Odor Descriptors

	Chemical Formula	Molecular Formula	Mw (g.mol ⁻¹)	Density (25°C)	bp (°C)	Odor descriptor ⁽²⁷⁾
ethyl acetate	C ₄ H ₈ O ₂		88	0.91	75	ethereal-fruity
ethyl butyrate	C ₆ H ₁₂ O ₂		116	0.90	121	fruity, pineapple
ethyl hexanoate	C ₈ H ₁₆ O ₂		144	0.89	168	fruity, banana, pineapple
2-pentanone	C ₅ H ₁₀ O		86	0.82	102	wine, acetone-like

The objective of this study was to determine the impact of the different components of the matrix on flavor retention in emulsions and complex media. To investigate the impact of functional groups and the carbon chain length of flavor compounds, a homologous series of ethyl esters (C₄, C₆, and C₈) and a ketone (C₅) were chosen. Thermodynamic properties of the four flavor compounds were measured in different matrices containing carbohydrates and/or lipids in order to quantify the degree of flavor compound retention and to understand better the effect of different components in a complex food matrix.

MATERIALS AND METHODS

Flavor Compounds. Four compounds, belonging to the strawberry flavor note (16) and with different physicochemical properties, were chosen: a homologous series of ethyl esters (C₄, C₆, and C₈) and a ketone (C₅). Degussa Flavors and Fruit Systems (Maxens, Grasse, France) kindly supplied them. Their purities were >98%. Their chemical formulas, molecular weights, densities, boiling points, and odor descriptors are presented in **Table 1**.

Preparation of Media. Mineral water in glass bottles (Volvic, Danone, France) was used throughout the study.

Lipid. Triolein [1,2,3-tri(*cis*-9-octadecenoyl)glycerol; 65% purity] was purchased from Sigma-Aldrich Chemie GmbH (Steinheim, Germany) and purified by percolation through a column packed with magnesium silicate (MgO:SiO₂ ≈ 15:85) of particle size 0.150–0.250 mm (60–100 mesh ASTM) (Floril, Merck, Darmstadt, Germany) (17). The purified triolein was stored at 4 °C.

Carbohydrate-Containing Matrix. A mixture containing waxy cornstarch (2.4% w/w; National Starch and Chemical, Villefranche, France), pectin (LM, DE = 30.5: 0.4% w/w; and HM, DE = 70.8: 0.9% w/w, Degussa Texturant Systems, Baupte, France), and D-glucose (1.8% w/w) was developed by Degussa Texturant Systems (Baupte, France). Citric acid (0.15% w/w, Prolabo, Paris, France), trisodium citrate (0.05% w/w, Prolabo), and tricalcium citrate (0.03% w/w, Sigma-Aldrich Chemie GmbH) were dissolved in mineral water under constant agitation with a magnetic stirrer; then the mixture of carbohydrates was added. The matrix was heated and boiled for 5 min and then cooled to a temperature of 35 °C. The rate of evaporation was controlled, and a solution of potassium sorbate (0.05% w/w, Degussa Texturant Systems) in mineral water was used to adjust the concentrations. This matrix was developed to have the same rheological properties as a liquid yogurt.

Lipid-Containing Matrices. Oil-in-water emulsions were prepared in batches of 100 mL by homogenizing liquid triolein (3.5% w/w) in

water containing soybean lecithin (0.4% w/w) as emulsifier (Emulpur N, Lucas Meyer GmbH, Hamburg, Germany) using an Ultra Turrax T25 homogenizer (Janke and Kunkel, IKA Labortechnik, Staufen, Germany) at a speed of 24000 rpm for 20 min.

The *complex matrix* containing lipids and carbohydrates was prepared as for the carbohydrate matrix. The amount of water was replaced by a similar quantity of the 3.5% oil-in-water emulsion. For the complex matrix, the carbohydrate concentration was the same as the carbohydrate matrix (5.5%, w/w) and the triolein concentration was the same as the oil-in-water emulsion (3.5%, w/w). Tricalcium citrate, which gives the carbohydrate matrix the desired rheological behavior, was not added to the complex matrix. The presence of triolein compensates for the rheological impact of this salt in the complex matrix.

Characterization of the Media. *Emulsion Characterization.* Viscosity was measured using a rotational viscometer Rheomat 30 (Contraves, Zurich, Switzerland) equipped with MSO coaxial cylinders and a Rheoscan 20 programmer. The measurements were performed at 37 ± 0.5 °C.

Particle size distribution was determined at ambient temperature using a Malvern Mastersizer laser diffractometer (Hydro 2000 G, Malvern Instruments, Orsay, France), both before and after headspace measurements to verify the stability of the emulsion.

Carbohydrate and Complex Matrix Characterization. *Rheological behavior* was measured before and after headspace measurements using a dynamic stress rheometer (SR 5000, Rheometric Scientific Inc., Piscataway, NJ) equipped with a cone-and-plate geometry cone (acrylic, 40 mm diameter, nominal cone angle of 0.04 rad, nominal gap of 0.0508 mm) heated at 37 °C by a Peltier system. A humidity cover trap was used to avoid the evaporation of water during the measurement. A shear stress sweep ranging from 1 to 160 Pa was applied, and the corresponding shear rate was measured. The flow curves giving shear stress σ (Pa) as a function of shear rate $\dot{\gamma}$ (s⁻¹) are characteristic of a shear-thinning behavior. The power law equation $\sigma = K\dot{\gamma}^n$ allows the calculation of the consistency index K and the flow behavior index n (Software RSI Orchestrator, v 6.3.2., Rheometric Scientific, 1997).

Determination of Flavor Compound Characteristics. Physicochemical characteristics of flavor compounds were measured or estimated.

Hydrophobicity. The log P value describes the partitioning of an organic compound between *n*-octanol and water. The hydrophobicity constants log P were estimated using a group contribution method (18). These values are the sum of the hydrophobic contributions of each functional group of the molecule.

Water Solubility. The solubility limit was measured using the mutual solubility method (19). In sealed flasks, an excess of the pure flavor compound was added to the water and allowed to equilibrate with gentle stirring at 37 ± 0.5 °C. After 24 h, the mixture was centrifuged with

Table 2. Physicochemical Characteristics of Carbohydrate and Complex Matrices

matrix	consistency index $K (\dot{\gamma} = 1 \text{ s}^{-1}) (\text{Pa}\cdot\text{s at } 37^\circ\text{C})$	flow behavior index n (at 37°C)	dry matter ^a (%)	A_w (25°C)	pH (25°C)	density ^b (g/mL) (25°C)
carbohydrate	0.81	0.59	5.3	0.990	3.53	1.204
complex	0.87	0.51	8.9	0.976	3.50	1.039

^a After 24 h in an oven at 102°C . ^b Measured by picnometry.

min at 4000 tr/min. Each system was repeated in triplicate. Analysis of the aqueous phase was carried out using a gas chromatograph CP3800 series (Varian Analytical Instruments, Walnut Creek, CA) fitted with an FID. The chromatograph was equipped with an automatic CombiPal injection system and a 1.5 m stainless steel column (2.2 mm internal diameter) packed with Chromosorb W-AW 100–200 mesh with a stationary phase of Carbowax 20M-10%. The operating conditions were as follows: nitrogen carrier gas flow rate, 25 mL/min; hydrogen flow rate, 33 mL/min; air flow rate, 330 mL/min; injector temperature, 190°C ; FID detector temperature, 200°C ; isothermal oven temperature, 90 or 100°C according to flavor compound. The chromatograms were registered and the data treated using Star Chromatography workstation software (v 5.31, Varian Associates, Inc., 1989–1998). Flavor compound concentrations in water (grams per liter) were determined using a standard calibration curve.

Saturated Vapor Pressure. The saturated vapor pressure, P_i^s (Pa) represents the volatility of the pure compound at a given temperature. It is an important factor in the partitioning of a chemical between air and water (20). The saturated vapor pressure values were calculated using the software MP.BPWIN (v 1.27, SRC, 1994–1997). Results were the mean values obtained by two methods using the boiling point: the Antoine method and the modified Grain method. This software gives accurate values for esters and ketones (21).

Measurements of Flavor Partitioning, Headspace Analysis. Flasks (20 mL) and aromatized matrices were pre-equilibrated at 37°C . Ten milliliters of aromatized matrices were placed in the flasks closed with a cap fitted with a Teflon-coated seal. These were placed in an incubator at $37 \pm 0.5^\circ\text{C}$. Preliminary experiments of headspace analysis at different equilibrium times were used to ensure that the analysis for each sample was performed at equilibrium. A time of 48 h was sufficient to reach equilibrium for each matrix and flavor compound. To verify that no flavor compounds were formed during the incubation time, blank samples (nonaromatized) of emulsions and carbohydrate and complex matrices were incubated and analyzed. For each flask (aromatized or nonaromatized), 1 mL of the vapor phase above the matrix was removed from the headspace with a thermostated gas syringe and injected into a FID gas chromatograph CP3800 series using the same conditions of analysis as described previously. The same batch of emulsions or matrices was used throughout an experiment. Each experiment was carried out at least three times using three different batches of each emulsion or matrix. The mass partition coefficient between gaseous phase and matrix was calculated as K_{mass} (eq 1):

$$K_{\text{mass}} = C_g / C_m \quad (1)$$

where C_g and C_m are the flavor mass fractions (w/w) in the gas and the matrix phase, respectively. Measurements were made at infinite dilution, where the partition coefficients are not influenced by the flavor compound concentration (50 ppm, v/w).

Liquid–Liquid Partition Coefficient. The flavor compound liquid–liquid partition was studied between mineral water and triolein. An aqueous solution containing flavor compound was in contact with purified triolein. The two phases were gently stirred at $37 \pm 0.5^\circ\text{C}$ until equilibrium was reached. After partitioning between triolein and water, the final flavor compound concentration in water was low; to ensure a good detection, different initial aqueous concentrations were chosen: ethyl acetate at 100 ppm (v/w), ethyl butyrate at 500 ppm, ethyl hexanoate at 1000 ppm, and 2-pentanone at 100 ppm. Analyses were carried out at least in triplicate. The aqueous phase was analyzed by a FID gas chromatograph CP3800 series. The equilibrium concentrations were determined with respect to a calibration curve, and the

liquid–liquid partition coefficient (P) was finally expressed as the ratio of the concentration (w/w) of flavor compound in oil and in water.

Vapor–Triolein Partition Coefficient. The flavor concentration in purified triolein was 500 ppm (v/w). The method of exponential dilution coupled with gas chromatography was used to measure the vapor–triolein equilibrium. An inert gas (nitrogen) passed through the liquid phase at a constant flow (30 mL/min) carried the flavor compound into the headspace. A sample of the vapor phase (1 mL) was automatically injected into the gas chromatograph at regular time intervals. Exponential dilution consists of exhausting the liquid phase of flavor compound in equilibrium with the vapor phase (22). Analyses were carried out on the FID gas chromatograph CP9000 (Chrompack Co., Middelberg, The Netherlands). The operating conditions of analyses were the same as for the CP3800, except the hydrogen and air flow rates were different: hydrogen flow rate, 25 mL/min; air flow rate, 250 mL/min. The chromatograms were registered and treated with Star Chromatography workstation software.

Statistical Analysis. Statistical analysis was carried out using Statistical Analysis System software (Procedure GML, SAS Institute, Inc., Cary, NC). A one-way analysis of variance followed by comparison of means by Student–Newman–Keuls test was applied to determine significant differences between the medium headspace concentrations. The significance level was $P < 0.05$ throughout the study.

RESULTS AND DISCUSSION

Characteristics of the Media. The rheological study indicated that the emulsion had a Newtonian behavior. At 37°C , the emulsion viscosity value was $0.94 \pm 0.07 \text{ mPa}\cdot\text{s}$. The water viscosity value at 37°C was $0.69 \text{ mPa}\cdot\text{s}$ (23), so the emulsion was slightly more viscous than water at the same temperature. Emulsion density was 0.997 g/mL at 25°C , and the pH value was 6.60. The average droplet size was $0.20 \pm 0.02 \mu\text{m}$; 80% of the droplets were between 0.09 and $0.90 \mu\text{m}$. Emulsions were stable: no aggregation was observed after headspace measurements, and the droplet size distribution of the emulsion was constant for at least 48 h.

The carbohydrate and complex matrices were prepared to have two matrices with similar rheological behaviors but with different compositions (with or without lipids). Physicochemical characteristics are given in **Table 2**. Both matrices present a strong shear-thinning behavior and similar consistency (K) and flow behavior (n) indices.

Characteristics of the Flavor Compounds. Partitioning of four flavor compounds from water, emulsions, and carbohydrate and complex matrices was studied. The flavor compounds differed considerably in physicochemical characteristics such as saturated vapor pressure, n -octanol–water partition coefficients ($\log P$), and water solubility (**Table 3**). Higher values of $\log P$ lead to a greater hydrophobicity, less solubility in water, and a higher affinity for triolein. Volatility of the pure component (P_i^s) decreased when the molar volume increased.

Flavor Partitioning. The partition coefficient K_{mass} between gaseous phase and matrix is dependent on different factors such as the water solubility, the saturated vapor pressure of the flavor compounds, the affinity for lipids, and the retention by carbohydrates (**Figure 1**). The behavior of flavor compounds

Table 3. Physicochemical Characteristics of Flavor Compounds

	molar volume (2θ) ^a ($\text{cm}^3\cdot\text{mol}^{-1}$)	$\log P(1\theta)$ ^a octanol/water (25 °C)	P^b triolein/water (mass fraction) (37 °C)	saturated vapor pressure ^c P^s (Pa) (37 °C)	water solubility ^d ($\text{g}\cdot\text{L}^{-1}$) (37 °C)
ethyl acetate	107	0.7	5	24527	67.1
ethyl butyrate	151	1.8	271	3839	5.3
ethyl hexanoate	196	2.8	2182	500	0.5
2-pentanone	121	0.8	4	9464	48.1

^a Estimated data. ^b Triolein/water partition coefficient, experimental data. ^c Estimated data, software MPBP-WIN, 1994–1997. ^d Experimental data.

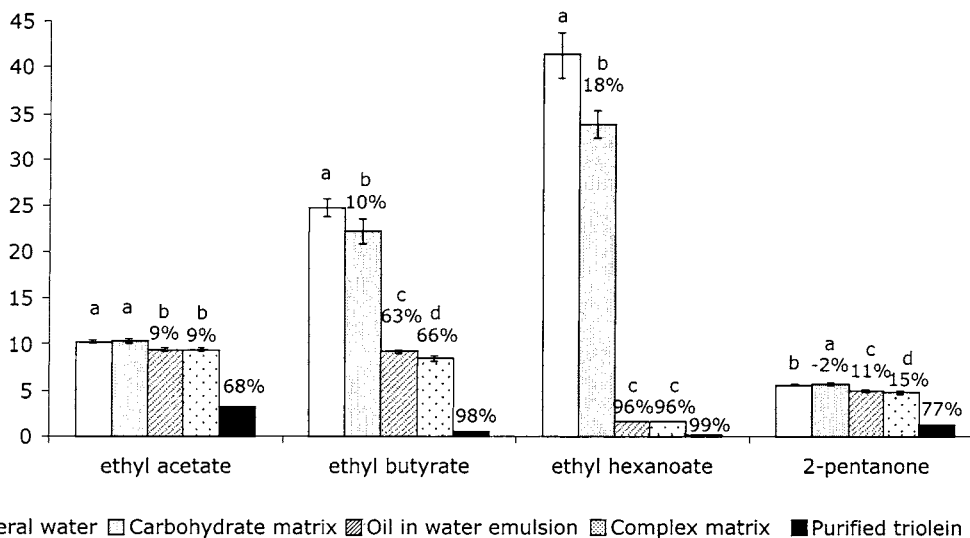


Figure 1. Partition coefficients (K_{mass}) of flavor compounds between gaseous phase and matrix. Different letters indicate that the results are significant at $P < 0.05$. A positive percentage value indicates a flavor compound retained by the matrix; a negative value indicates a flavor compound released by the matrix.

was investigated in simple matrices (mineral water and purified triolein) and in food model media (such as an oil-in-water emulsion, a carbohydrate matrix, and a complex matrix).

Simple Media. In water, for the homologous series of ethyl esters, the more hydrophobic compound was the more volatile (Figure 1). This result is in agreement with the literature. The same tendency was found at 25 °C by Landy et al. (24).

Ethyl butyrate and ethyl hexanoate solubilities in water were low due to their hydrophobic character. They were also only slightly volatile according to their saturated vapor pressure, due to their molar volume (Table 3). Hence, their volatility from water was high (Figure 1). Hydrophobic molecules have little affinity for water molecules but have a great affinity for lipids. The affinity of ethyl butyrate for lipids is 271 times greater than for water, and ethyl hexanoate has an affinity for lipids that is 10 times that of ethyl butyrate (Table 3). Increasing the carbon chain length leads to greater solubilization in the triolein.

Ethyl acetate solubility in water was greater than 2-pentanone solubility; however, the saturated vapor pressure of ethyl acetate was greater than the saturated vapor pressure of 2-pentanone (Table 3). As a result, ethyl acetate was more volatile from water than 2-pentanone (Figure 1). However, partition coefficients P between triolein and water show that their affinities for triolein were similar (Table 3). These flavor compounds have similar molecular weights and $\log P$ values, but their behaviors in the presence of water are very different. The only difference between these two compounds is the substitution of a carbon atom by an oxygen atom (Table 1), but this difference in functional group has led to a different flavor compound behavior.

Food Model Media. The objective of using two matrices with the same rheological behavior but with different compositions

was to determine the influence of the matrix composition on the flavor compounds behavior, principally their retention by the matrix. The calculated percentage of flavor compound retained with reference to the water matrix was used to indicate the degree of interactions between the flavor compound and the matrix components.

The flavor compound retention percentage was calculated using the following formula (eq 2):

$$R = \frac{K_{\text{mass}}^{\text{water}} - K_{\text{mass}}^{\text{matrix}}}{K_{\text{mass}}^{\text{matrix}}} \times 100 (\%) \quad (2)$$

A positive percentage value indicates a flavor compound retained by the matrix, and a negative value indicates a flavor compound released by the matrix (Figure 1).

The ratio between two partition coefficients allows a comparison of the effect of different components on flavor retention, in particular, the effect of lipid and carbohydrate both separately and in combination (Table 4). The ratio between water K_{mass} and carbohydrate matrix K_{mass} or between emulsion K_{mass} and complex matrix K_{mass} shows the effect of the polysaccharide. The ratio between water K_{mass} and emulsion K_{mass} or between polysaccharide matrix K_{mass} and complex matrix K_{mass} shows the effect of the lipid. The ratio between water K_{mass} and complex matrix K_{mass} shows both the carbohydrate and lipid effects. When the ratio value is >1 , there is a significant component effect on flavor retention.

Lipid Effect. A comparison of flavor compound volatility from matrices containing fat (3.5% oil-in-water emulsion, complex matrix, and triolein) and from water showed that fat added to the matrix leads to a decrease in the concentration in the gaseous

Table 4. Ratio of Partition Coefficients, K_{mass} , for Flavor Compounds in the Different Matrices

$K_{\text{mass}} \text{ matrix}/$ $K_{\text{mass}} \text{ matrix}$	ethyl acetate	ethyl butyrate	ethyl hexanoate	2-pentanone
water/carbohydrate	1.0 ^a	1.1 ^a	1.2 ^a	0.9 ^a
water/emulsion	1.1 ^a	2.7 ^a	25.1 ^a	1.1 ^a
water/complex	1.1 ^a	2.9 ^a	25.1 ^a	1.2 ^a
emulsion/complex	1.0 ^a	1.1 ^a	1.0 ^a	1.1 ^a
carbohydrate/complex	1.1 ^a	2.6 ^a	20.5 ^a	1.2 ^a

^a Significant with a level of 5%.

phase for all flavor compounds. If we consider the homologous series of ethyl esters, retention was more important when the number of carbon atoms increased, that is, when hydrophobicity increased. According to the triolein/water partition coefficients, ethyl butyrate and ethyl hexanoate have higher affinities for triolein than ethyl acetate and 2-pentanone (Table 3). This behavior was the reverse of the flavor compound solubility in water. These compounds were more soluble in the lipid phase than in water (Table 3). Hence, their partial vapor pressure and, consequently, their concentration in the headspace decreased.

When flavor compounds were added to purified triolein, the percentage retention decreased in the following order: ethyl hexanoate (99%), ethyl butyrate (98%), 2-pentanone (77%), and ethyl acetate (68%) (Figure 1). Due to their somewhat higher polarity, ethyl acetate and 2-pentanone were less retained by lipids than ethyl butyrate and ethyl hexanoate.

A retention effect by lipids is well-known (8, 25). An impact of lipids in emulsions or in a complex matrix on flavor compound retention was significant for all of the compounds (Table 4). Carey et al. (26) showed an effect of cloud emulsion on flavor compound retention even at low fat concentrations (<0.2%), with less effect on ethyl butyrate and more effect on ethyl octanoate and octanone.

Carbohydrate Effect. This study also shows a global carbohydrate effect on flavor retention. The retention of flavor compounds depends on a combined effect of sucrose, pectin, and starch. A comparison of flavor compound volatility from water and from carbohydrate matrix shows that the retention increases with molecular weight for ethyl butyrate (10%) and ethyl hexanoate (18%); no retention for ethyl acetate and a small effect of release (-2%) were observed for 2-pentanone (Figure 1). In this case, adding carbohydrates seems to decrease the availability of water for the solubilization of 2-pentanone and, hence, volatility increases.

The ratio between water K_{mass} and carbohydrate matrix K_{mass} showed a significant effect of retention by carbohydrates on both ethyl butyrate (1.1) and ethyl hexanoate (1.2).

Carbohydrate Effect in the Presence of Lipids. In the complex matrix there was 3.5% of triolein and 5.5% of carbohydrates. The lipid effect on retention was dominant compared with the carbohydrate effect. For ethyl hexanoate, the most hydrophobic molecule, the ratio water K_{mass} /emulsion K_{mass} (25.1) or water K_{mass} /complex matrix K_{mass} (25.1) was greater than water K_{mass} /carbohydrate matrix K_{mass} (1.2). However, a carbohydrate effect on flavor compound retention even in the presence of lipids was demonstrated for two compounds. For both ethyl butyrate and 2-pentanone, the ratio carbohydrate matrix K_{mass} /complex matrix K_{mass} value was 1.1, showing a significant carbohydrate effect in the presence of lipids. For ethyl hexanoate in the presence of lipids the effect of carbohydrate on retention was masked by the impact of lipid retention. For ethyl acetate, the

flavor compound most hydrophilic and soluble in water, the retention seems to be governed by the water and carbohydrates or lipids have little effect on retention.

Conclusion. At thermodynamic equilibrium, the partition between gaseous phase and matrix of the flavor compounds is dependent on their physicochemical characteristics, principally their hydrophobicity. Flavor compound retention by matrices shows that physicochemical interactions occur between matrix components and flavor molecules. This suggests that changes in matrix composition could lead to different flavor partitions in multiphase foods. A lipid effect on retention was shown for all of the matrices and for each flavor compound. A carbohydrate effect on retention was also shown in the presence of lipids for two flavor compounds: ethyl butyrate and 2-pentanone. These results will be completed by a kinetic study to determine the carbohydrate and/or lipid effect on the flavor release as a function of time.

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