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Partition coefficients of aroma compounds in polysaccharide solutions by the phase ratio variation method

Céline Jouquand, Violette Ducruet, Pierre Giampaoli*

ENSIA, UMR-SCALE, Département Science de l'Aliment, 1 av. des Olympiades, 91744 Massy, France

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Abstract

The partition coefficients (*K*) of aroma compounds (a homologous series of ketones, hexanal, *t*–2-hexenal, ethyl butanoate and 1-hexanol) in polysaccharide solutions were determined by the phase ratio variation method (PRV method) using a headspace autosampler. This method enabled easy determination of the partition coefficients of volatile compounds in a gas/liquid system without external or internal calibration, and the results agreed well with published data obtained by direct method. Measurements of *K* at different temperatures enabled the investigation of aroma compound retention by maltodextrin and β-cyclodextrin during heat treatment. In a maltodextrin solution, retention depended on the hydrophobicity of aroma compounds and it was favoured by the increase of temperature (from 60 to 80 °C). In a β-cyclodextrin solution, temperature variations produced different effects on the retention of aroma compounds and could reveal differences in the nature of the interaction with β-cyclodextrin.

Keywords: Static headspace; Partition coefficient; Aroma compounds; Maltodextrin; β-Cyclodextrin; Phase ratio variation (PRV) method

1. Introduction

Polysaccharides are widely employed in the cereal industry and as thickening and stabilizing agents in sauces, soups or drinks. Starch and its derived products like maltodextrins and β-cyclodextrin are also known to encapsulate aroma compounds and interactions between aroma compounds and these polysaccharides have been the subject of considerable studies (Goubet, Le Quéré, & Voilley, 1998; Reineccius, 1991). During thermal treatment (cooking, pasteurization), some aroma compounds of food matrices can be lost (Prost, 1994). The addition of maltodextrins and β-cyclodextrin as stabilizing or thickening agents could retain some aroma compounds in food matrices during these thermal processes.

In model systems, polysaccharides generally induce a reduction in aroma release caused by an increase in viscosity and/or by molecular interactions with flavour compounds. One way of investigating the retention (or release) of aroma compounds by polysaccharides is to measure the gas/liquid partition coefficient *K*. This parameter describes the distribution of volatile compounds between the gas phase and the food matrix. Both static methods (headspace analysis) and dynamic methods (exponential dilution)—have been used to measure this partition coefficient. In the latter case, the amount of aroma compounds in the gas phase decreases exponentially as a function of time; this time-related change follows an exponential law and enables fast determination of the partition coefficient (Langourieux & Crouzet, 1994; Sadafian & Crouzet, 1987). The static method requires measurement of the aroma compound concentration in each phase by gas chromatography when the gas/solution equilibrium is reached (Cayot, Taisant, Arvisenet, Meunier, & Voilley, 2000; Nahon, Harrison, & Roozen, 2000). This method appears to be more tedious than exponential dilution, and the concentration of aroma compounds in the liquid phase is not always measured directly (Salvador, Bakker, Langley, Potjewijd, Martin, & Elmore, 1994).

Another static method was proposed to establish the partition coefficient of benzene, toluene, chlorobenzene and 2-butanone in a gas/liquid system without the need to measure the volatile compound concentration in both phases (Ettre & Kolb, 1991; Ettre, Welter, & Kolb, 1993). This phase ratio variation method (PRV) uses an automatic headspace sampler coupled to a gas chroma-

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* Corresponding author. Tel.: +33-1-69-93-50-23; fax: +33-1-69-93-50-20.

E-mail address: giamp@ensia.inra.fr (P. Giampaoli).

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tograph and is based on the relationship between K and the phase ratio (ratio of gas and liquid phases volumes). This technique was successfully applied in environmental field to measure the Henry's constants of volatile organic compounds (VOCs) and it was validated by the authors comparing their data with literature data (Peng & Wan, 1997, 1998). The main advantage of the PRV method is the lack of external or internal calibration which creates many drawbacks widely described by Chaintreau, Grade, and Muñoz-Box (1995).

The objectives of this work were first to demonstrate that the PRV method is suitable for determining the partition coefficients of aroma compounds in a gas/liquid system in food field and secondly to apply this method to the retention of aroma compounds by polysaccharides during heat treatment.

2. Material and methods

2.1. Reagents

Ethyl butanoate, 2-heptanone, 2-hexanone and 1-hexanol were obtained from Ega (France); *t*–2-hexenal, hexanal and 2-octanone came from Aldrich (St. Quentin Fallavier, France) and 2-butanone was obtained from Acros Organics (Noisy-Le-Grand, France). The physicochemical properties of these aroma compounds are shown in Table 1. Maltodextrin DE 5 with 1% amylose (Glucidex 6) and β-cyclodextrin (Kleptose) were provided by Roquette Frères (Lestrem, France).

2.2. Phase ratio variation method

The original sample solution is defined by V_s, m_s and C_s where

V_s = volume of the original sample solution introduced into the sample vial, m_s = the mass of the volatile compound in the original sample and C_s = the initial concentration of the volatile compound in the original sample expressed as mass per volume

$$C_S = m_S/V_S \qquad (1)$$

We can also express the phase ratio (β) of the vial containing the sample

$$\beta = V_G/V_S \qquad (2)$$

The reciprocal of the partition coefficient K can be expressed as:

$$\mathrm{K} = C^*_S/C^*_G \qquad (3)$$

where C^*_S = concentration of the volatile compound in the liquid phase at equilibrium, C^*_G = concentration of the compound in the gas phase at equilibrium.

Defining the two concentration as

$$C^*_S = m^*_S/V_S \qquad (4)$$

$$C^*_G = m^*_G/V_G \qquad (5)$$

the partition coefficient can be expressed as:

$$\mathrm{K} = \frac{C^*_S}{C^*_G} = \frac{m^*_S}{m^*_G} \cdot \frac{V_G}{V_S} = \frac{m^*_S}{m^*_G} \cdot \beta \qquad (6)$$

we can express m_S as

$$m_S = m^*_S + m^*_G \qquad (7)$$

$$\frac{m_S}{V_S} = \frac{m^*_S}{V_S} + \frac{m^*_G}{V_S} \qquad (8)$$

but $V_S = V_G/\beta$ therefore,

$$\frac{m_S}{V_S} = \frac{m^*_S}{V_S} + \frac{m^*_G}{V_G} \cdot \beta \qquad (9)$$

$$C_S = C^*_S + C^*_G.\beta \qquad (10)$$

also, since $C^*_S = \mathrm{K}.C^*_G$, so,

$$C_S = \mathrm{K}.C^*_G + C^*_G.\beta = C^*_G\ [\mathrm{K} + \beta] \qquad (11)$$

Table 1
Physicochemical properties of aroma compounds

Aroma compounds	Purity (%)	Density	mol wt.	Saturated vapour pressure at 25 °C (mm Hg)	Solubility in water at 25 °C (g/l)	Log *P*
Hexanal	98	0.830	100	11.26[a]	4.8[b]	1.78[a]
2-Octanone	98	0.819	128	1.35[a]	1.2[c]	2.37[a]
Ethyl butanoate	99	0.878	116	17.3[d]	5.6[d]	1.70[d]
2-Heptanone	98	0.820	114	3.85[a]	4.3[a]	1.98[a]
2-Hexanone	98	0.812	100	11.6[a]	20[b]	1.38[a]
t–2-Hexenal	98	0.846	98	6.6[a]	5.3[a]	1.58[a]
2-Butanone	98	0.810	72	90.6[a]	22.3[a]	0.29[a]
1-Hexanol	99	0.814	102	0.928[a]	5.9[a]	2.03[a]

[a] Syracuse Research Corporation (2002).
[b] Chemexper Chemical Directory (2002).
[c] Estimated value, Grant and Higuchi (1990).
[d] Le Thanh, Lamer, Voilley, and Jose (1993).

From this equation C_G^* can be expressed as

$$C_G^* = \frac{C_S}{K + \beta} \tag{12}$$

this equation has been established by Ettre and Kolb (1991).

Taking the reciprocals of both sides, Eq. (12) becomes:

$$\frac{1}{C_G^*} = \frac{K}{C_S} + \frac{1}{C_S} \cdot \beta \tag{13}$$

in headspace analysis, the peak area is proportional to the equilibrium concentration in the headspace of vials:

$$A = fi.C_G^* \tag{14}$$

A = peak area obtained by analyzing an aliquot of the gas phase of the sample vial, at equilibrium; fi = proportional factor.

Substituting A/fi for C^*_G into Eq. (13):

$$\frac{1}{A} = \frac{K}{fi \cdot C_S} + \frac{1}{fi \cdot C_S} \cdot \beta \tag{15}$$

this relationship has been established by Ettre et al. (1993).

Using a sample solution with C_S as the sample concentration and testing increasing volumes (V_S) in different headspace vials, we could assume that K and C_S were the same in each vial, at a given temperature. The only variables were the phase ratio (β) and the peak area (A). Thus, Eq. (15) corresponds to a linear equation of the following type:

$$1/A = a + b.\beta \tag{16}$$

where $a = K/(fi.C_S)$ and $b = 1/(fi.C_S)$

$$K = a/b \tag{17}$$

K is calculated from the values of a and b obtained by plotting 1/A against β.

As an example, Table 2 lists the raw data, the linear regression and calculated K obtained for hexanal at 60 °C.

All our data were inverted ($K = C^*_S/C^*_G \rightarrow K = C^*_G/C^*_S$) in order to facilitate the comparison with published data.

2.3. Retention of aroma compounds by polysaccharides

The partition coefficients of eight aroma compounds were determined by the PRV method in different matrices (water, β-cyclodextrin, and maltodextrin DE 5 with 1% amylose), at three temperatures: 60, 70 and 80 °C. For each matrix and each aroma compound, K measurements were done in triplicate. Partition coefficients of 2-heptanone, 2-octanone, hexanal and ethyl butanoate in water were also measured at 25 °C in order to compare with published data.

The gas/liquid partition coefficients of aroma compounds in water were chosen as the references and enabled determination of the percentage of retention (r) of the aroma compound by polysaccharide.

$$r(\%) = \left[1 - \frac{K_{\text{polys.}}}{K_{\text{water}}}\right] \times 100 \tag{18}$$

2.4. Sample preparation

Maltodextrin or β-cyclodextrin was added to distilled water to respectively obtain a final concentration of 10% (w/w) and 1% (w/w). Then, the polysaccharide aqueous solutions were manually homogenized during 2–3 min at ambient temperature.

Pure aroma (5 μl) was introduced in 200 ml of maltodextrin aqueous solution or 200 ml of β-cyclodextrin aqueous solution. An aqueous solution without polysaccharides was also prepared. Polysaccharide solutions were stored 1 h at ambient temperature before headspace analysis. Then, increasing volumes (1, 2, 3 and 4 ml) of each aqueous solution were poured into headspace vials (22 ml); thus, each vial represented a different phase ratio β (21; 10; 6.3; 4.5).

2.5. Instrumentation

Measurements of the gas phase in the sample vials were performed using an Automatic Headspace Sampler (Perkin-Elmer model HS 40XL) coupled to a gas chromatograph with a flame-ionization detector (Perkin-Elmer model AutoSystem XL). The samples were thermo stated at the given temperature during 80 min without agitation. Preliminary experiments of headspace analysis at different times for each aroma compound showed that at 60 min, equilibrium was reached. Pressurization time was 2 min and sample injection time was 0.05 min. The gas used to pressurize the samples was helium.

A capillary DB5 column (J&W Scientific) was employed (length: 25 m, internal diameter: 0.32 mm, film thickness: 0.52 μm). The conditions for gas chromatography were as follows: oven temperature program: from 100 to 150 °C at a rate of 12 °C/min. The carrier gas was helium at a flow rate of 1.8 ml/min. Detector and injector temperature was 250 °C. For the FID detector, air and H_2 flow rates were 450 and 45 ml/min, respectively.

3. Results and discussion

3.1. PRV method

In order to compare PRV method used in this work to direct method, partition coefficients of four aroma

Table 2
Data for aqueous solution of hexanal at 60 °C

Temperature	Volume of solution in vial (ml)	Phase ratio β	Peak area (average of three sets vials)	Slope b	Intercept a	Correlation coefficient R^2	Partition coefficient $K = C_S^*/C_G^*$
60 °C	1	21	162 490	1.85×10^{-7}	2.25×10^{-6}	0.998	12.2
	2	10	248 906				
	3	6.3	291 089				
	4	4.5	319 826				
60 °C	1	21	165 605	1.85×10^{-7}	$2\times14\times10^{-6}$	0.998	11.6
	2	10	253 887				
	3	6.3	306 536				
	4	4.5	328 689				
60 °C	1	21	148 967	2.02×10^{-7}	2.45×10^{-6}	0.999	12.1
	2	10	225 320				
	3	6.3	269 767				
	4	4.5	293 002				

compounds were measured at 25 °C. According Table 3, partition coefficients determined by the PRV method were very closed to those measured by the direct method. In comparison with the direct method, the main advantage of the PRV method was the lack of external or internal calibration. Indeed, the measure of partition coefficient by direct method needs to extract the aroma compound remaining in the solution at equilibrium and in parallel to determine the concentration of the aroma compound in the gas phase. In practice, the procedure is variously simplified: (i) the liquid/liquid extraction is rarely made (Cayot, et al., 2000) and the concentration of the aroma compound in solution at equilibrium is often approximated by the following equation (Jung & Ebeler, 2003; Nahon et al., 2000):

$$C_S^* = C_S - C_G^*(V_G/V_S) \tag{19}$$

(ii) the concentration of the aroma compound in the gas phase is often established using external calibration curve of the compound in a solvent and not by dilution of the aroma compound in vapour state. So the procedure of the direct method varied according the different authors. The results reported by Voilley (1999) showed great variations of partition coefficients of aroma compounds in water obtained by the direct method. As an example, K of 2-nonanone in water, at 25 °C, varied to 7.7×10^{-3} to 35×10^{-3}.

Pressurization prior to injection could modify the accuracy of partition coefficient calculations. Chaintreau et al. (1995) reported that the values of K obtained with pressurization of the sample were higher than in systems operating at atmospheric pressure, essentially for solvent like hexane. Preliminary experiments on ethyl butanoate in water showed that the value of K was not modified when two different pressures in the headspace vial were tested (1.5 and 2 atm.) Moreover, in Table 3, the values of K obtained by the PRV method are very closed to those obtained by the direct method. So, pressurization seemed to have a weak impact on the determination of K of aroma compounds in this work.

Ettre et al. (1993) showed that the accuracy of partition coefficient calculations could be improved by large differences in peak area values, resulting from changing the phase ratio values. Large differences in peak area values are obtained for relatively nonpolar compounds, which are easily released in the gas phase. As for polar molecules, the relative area differences become smaller as the K increased. These authors reported that for low gas/liquid partition coefficients ($<1.10^{-2}$), the accuracy of measurements would be poorer which represents the limitation for the use of the PRV method. In their paper dealing with the influence of the sample volume in the equilibrium headspace, Ettre and Kolb (1991) calculated that for a low partition coefficient (4×10^{-3}), variation of concentration of volatile compound in the gas phase will be only of 1% when β decreases from 4 to 0.25. For a partition coefficient of 1, variation will be of 75% when β decreases from 4 to 0.25. So, the influence of the sample volume was important only in the case of high partition coefficients ($>1.10^{-2}$). In our study, all aroma compounds had a partition coefficient greater than 1.10^{-2} except for 1-hexanol at 60 °C ($K=8.5\times10^{-3}$).

3.2. *Partition coefficients of aroma compounds in water*

The partition coefficients of the eight aroma compounds were determined in water, at three different temperatures (Table 4). At each temperature, the headspace of the aqueous solution was analyzed from vials with different phase ratios. Linear regression analysis was performed according to Eq. (16) and the partition coefficient K was calculated using Eq. (17).

The air/water partition coefficients of aroma compounds were representative of the volatility of these molecules in water. At the three studied temperatures, hexanal appeared to be the most volatile compound in water and 1-hexanol was the less volatile compound. The behaviour of volatile compounds in water can be explained by their physicochemical properties. Indeed, for partially soluble compounds (less than 10 g/l), Amoore and Buttery (1978) established a relationship giving their partition coefficients in water based on their saturated vapour pressure, their solubility in water and their molecular weight. Table 3 compares the partition coefficients in water at 25 °C, for four compounds, measured by the PRV method with the results calculated by the Amoore and Buttery model. The agreement was quite satisfactory.

For the homologous series of ketones, there was a linear relationship between log K and the number of carbon atoms (Fig. 1). This result agrees with the findings of other authors (Buttery, Ling, & Guadagni, 1969; Landy, Druaux, & Voilley, 1995). This phenomenon results from a reduction in the polar character of compounds when the carbon chain length increases, i.e. Log P increases as K increases.

The effect of temperature on the partition coefficients of volatile compounds was previously studied by Carelli, Crapiste, and Lozano (1991), Ettre et al. (1993), Kieckbush and King (1979), and Kolb, Welter, and Bichler (1992). The relationship between log K and $1/T$ may be considered as linear, and investigation of the validity of this relationship may provide a check on the correctness of the data measured. Fig. 2 shows the plots for hexanal, ethyl butanoate, 2-octanone and 2-heptanone. Additional partition coefficient measurements were performed at 25 and 40 °C to validate this relationship. 2-Octanone, hexanal and ethyl butanoate seemed to exhibit the same behaviour in water and 2-heptanone appeared to be less volatile than the other three compounds in water.

3.3. Interactions between aroma compounds and polysaccharides

In Fig. 3, the partition coefficients of aroma compounds are given in water and in a maltodextrin solution at 80 °C. The presence of maltodextrin influenced the partition coefficients of these compounds and allowed us to calculate the percentage of retention according to Eq. (18). The retention of aroma compounds by a maltodextrin solution, at three temperatures, is shown in Fig. 4. The most retained compounds were hexanal, 2-octanone, ethyl butanoate and 2-heptanone.The retention of aroma compounds seemed to be linked to the hydrophobicity of aroma compounds

Table 3
Air/water partition coefficient ($\times 10^2$) of aroma compounds at 25 °C measured by different methods

Aroma compounds	PRV method	Direct method in static headspace	Model of Amoore and Buttery
Hexanal	1.1	0.87[a]	1.26
Ethyl butanoate	1.8	1.83[b]	1.93
2-Heptanone	0.57	0.59[a]	0.55
2-Octanone	0.62	0.77[a]	0.77

[a] Buttery et al. (1969).
[b] Le Thanh et al. (1993).

Table 4
Air/water partition coefficient ($\times 10^2$) of aroma compounds at different temperatures

Aroma compounds	60 °C	70 °C	80 °C
Hexanal	8.33±0.2	12.7±0.5	18.9±2
2-Octanone	7.46±0.4	12±1.9	18.5±1.5
Ethyl butanoate	8±0.16	12.4±0.6	16.7±0.7
2-Heptanone	3.9±0.16	7.14±0.34	10.3±0.2
2-Hexanone	2.9±0.16	4.35±0.36	5.99±0.3
t-2-Hexenal	2.13±0.1	2.76±0.2	3.34±0.1
2-Butanone	1.0±0.06	1.63±0.05	2.36±0.02
1-Hexanol	0.85±0.06	1.33±0.05	2.02±0.2

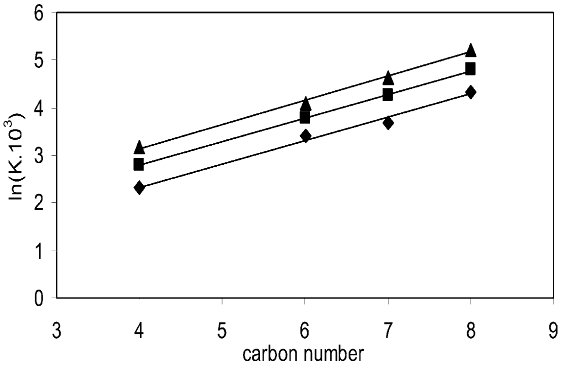

Fig. 1. Air/water partition coefficients at 60 °C (◆), 70 °C (■) and 80 °C (▲) for a homologous series of ketones vs. carbon number.

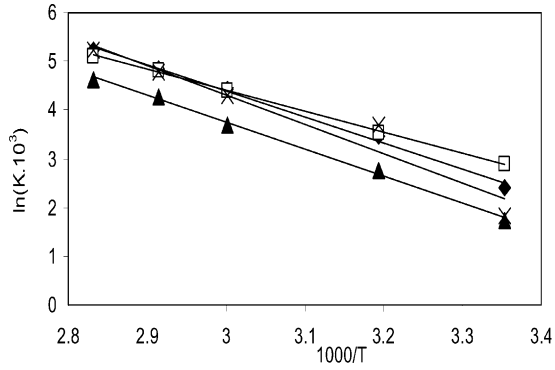

Fig. 2. Logarithm of partition coefficient vs. reciprocal of absolute temperature ($1/T$) for hexanal (◆), 2-octanone (×), 2-heptanone (▲) and ethyl butanoate (□) in air/water system.

except for 1-hexanol. Maltodextrin molecules in water can regroup themselves to create a local hydrophobic medium and then organize the water molecules between them (Druaux, Le Thanh, Seuvre, & Voilley, 1998). Thus hydrophobic molecules such as hexanal, 2-octanone, ethyl butanoate and 2-heptanone introduced in such a solution could interact with maltodextrin because of the lack of strong favourable interactions with water molecules (Dubois, Lubbers, & Voilley, 1995). Kieckbush and King (1979) reported that pentyl acetate, a nonpolar molecule relatively volatile in water was retained in the liquid phase containing maltodextrin.

2-Butanone exhibited negative retention at 60 and 70 °C, i.e. release of this compound in the gas phase. This effect could be assimilated to a salting-out phenomenon. In the presence of maltodextrin, competition to bind water molecules occurred with 2-butanone (a polar molecule), and led to a release of the aroma compound in the gas phase. The same behaviour was reported by Kieckbush and King (1979) for polar acetate (ethyl acetate, propyl acetate and butyl acetate). 2-Butanone and 1-hexanol exhibited the same behaviour at 60 °C. In spite of its relatively high hydrophobicity (Log $P = 2.03$), 1-hexanol has a hydroxyl group which may interact with water molecules through H-bonds. So, there was a competition between maltodextrin and 1-hexanol to bind water molecules, which explained its negative retention.

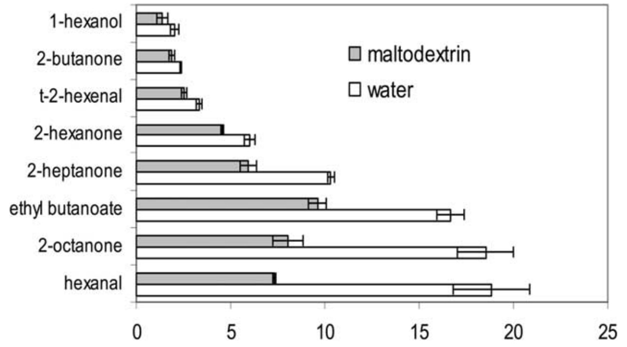

Fig. 3. Partition coefficients ($\times 10^2$) of aroma compounds in water and in a maltodextrin solution at 80 °C.

Nevertheless, retention of 1-hexanol and 2-butanone became positive respectively at 70 and 80 °C, and for all the studied compounds, percentage of retention increased with a rise in temperature. This increase of temperature decreasing the strength of hydrogen bonds could favour the hydrophobic effect. This effect was shown by Kieckbush and King (1979): the percentage of retention of pentyl acetate in maltodextrin solution (23.9%, w/w) increased from 3.4 to 12.4% with the rise in temperature from 25 to 45 °C.

Fig. 5 shows the retention of aroma compounds by a β-cyclodextrin solution. 2-octanone was the most markedly retained molecule and its greater retention could be closely linked to its high hydrophobicity (Log $P = 2.37$). In solution, β-cyclodextrin exhibits a preference for complexing with the most hydrophobic compounds present (Pagington, 1985). In our study, this behaviour only applied to aroma compounds with a linear carbon chain. Ethyl butanoate, which has an angled chemical function, showed less retention despite its relatively high hydrophobicity (Log $P = 1.70$). This compound was half as retained as molecules with similar hydrophobicity (hexanal and 2-heptanone). Because of its angled chemical function, the molecular volume of ethyl butanoate may be greater than that of hexanal and 2-heptanone and thus may limit its inclusion in the inner cavity of β-cyclodextrin (Goubet, Dahout, Sémon, Guichard, Le Quéré, & Voilley, 2001).

A salting-out phenomenon occurred at 60 and 70 °C in β-cyclodextrin solution for 2-butanone and this behaviour was comparable with that seen in the maltodextrin solution.

Unlike the maltodextrin solution, temperature had different effects on the retention of aroma compounds by β-cyclodextrin. The increase of temperature to 80 °C allowed the retention of 2-butanone by β-cyclodextrin due to hydrophobic interactions while at lower temperatures, the H-bonds between water and 2-butanone were more favourable.

For hexanal, ethyl butanoate, 2-octanone, 2-heptanone and 2-hexanone, the percentage of retention did

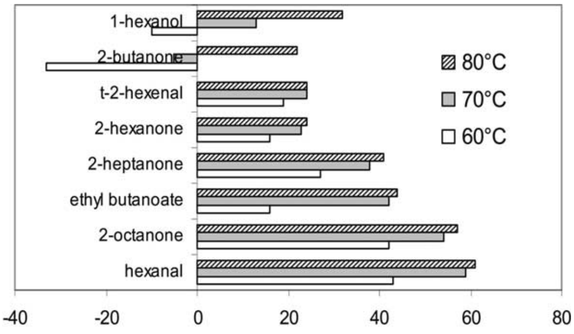

Fig. 4. Percentage of retention of aroma compounds in a maltodextrin solution (10%, w/w).

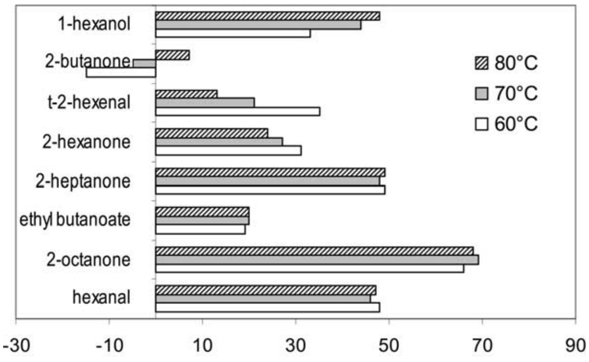

Fig. 5. Percentage of retention of aroma compounds in a β-cyclodextrin solution (1%, w/w).

not vary with temperature. It can be assumed that the hydrophobic portion of these molecules or their whole carbon chain was included in the inner cavity of β-cyclodextrin and that the increase in temperature had no effect on the stability of these complexes.

At 60 °C, the retention of 1-hexanol was low (33%) compared with hydrophobic compounds like hexanal and 2-heptanone. This phenomenon could be due to the hydroxyl group of this compound which could interact with water through H-bonds. At 80 °C, the retention reached 48% like hexanal (47%) and 2-heptanone (49%) and could be explained by the high hydrophobicity of this compound (Log $P = 2.07$). So, the temperature seemed to influence the nature of interactions between 1-hexanol and β-cyclodextrin.

In the case of *t*–2-hexenal, the percentage retention decreased as the temperature rose. This compound may be retained on the outer surface of β-cyclodextrin which is lined by hydroxyls groups capable of interacting with *t*–2-hexenal through H-bonds. Thus, as the strength of the H-bonds decreased with the rise in temperature, the interactions between *t*–2-hexenal and β-cyclodextrin were reduced at higher temperatures.

4. Conclusion

The interactions between aroma compounds and polysaccharides were studied by the phase ratio variation method using a static headspace autosampler. This is a convenient methodology to determine the partition coefficients of aroma compounds in a gas/liquid system and the results agreed well with published data obtained by the direct method in static headspace. The main advantages of this method are its good repeatability and the lack of external or internal calibration which is tedious, or in many cases, not very appropriate for food matrices.

The retention of aroma compounds by polysaccharides was studied with variations of temperature. The effect of temperature influenced and revealed the nature of interactions between aroma compounds and polysaccharides. In the maltodextrin solution, an increase in temperature favoured the retention of all aroma compounds by hydrophobic effect. In the β-cyclodextrin solution, hydrophobic compounds established an energetically favourable nonpolar–nonpolar interaction with the inner cavity of β-cyclodextrin. For polar compounds like *t*–2-hexenal, temperature variations decreased the retention by β-cyclodextrin.

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