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# Determination of partition coefficient of migrants in food simulants by the PRV method

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**Abstract**

Partition coefficients of six migrants between four simulated foods (water, 10% ethanol, 3% acetic acid, 95% ethanol) and air were determined by the phase ratio variation (PRV) method using headspace analyses by gas chromatography. The migrants were ethyl acetate, methyl ethyl ketone, propyl alcohol, butyraldehyde, acetaldehyde and acetonitrile. The results showed that migrant absorption by the four food simulants was highly dependent on the physicochemical properties of migrants and foods, such as polarity, solubility and hydrogen-bonding.


*Keywords:* Partition coefficient; Polarity; Solubility; Phase ratio variation

## 1. Introduction

Printing on food packaging (involving solvent use) is widespread in the food industry to inform and attract consumers. However, migration of residual printing ink solvents from packaging to food can cause off-flavours in food and lead to a deterioration in the quality of the food products (Gilbert, 1976; Mc Gorrin, Pofahl, & Croasmun, 1987; Piringer, 1986).

Solvents consist of low molecular weight compounds, such as hydrocarbons, alcohols, ketones and esters (Kumai et al., 1983) which can migrate into food.

Several studies have reported partition coefficients of solvents between various foods and air (An & Halek, 1995; Halek & Hatzidimitriu, 1988; Heydanek, Woolford, & Baugh, 1979) and these involved finding factors that affected the partition coefficients of solvents in food/air systems (Halek & Levinson, 1988, 1989; Halek & Chan, 1994).

Analysis of all the mass transport processes in a real food-packaging system is very complex. For this reason, the system is simplified and each transferable compound is analysed separately. The package is assumed to be homogeneous, the food is substituted by a suitable simulant and the substance to be analysed is introduced at a known concentration.

Aqueous, acidic or alcoholic foodstuffs are well simulated by distilled water, 3% acetic acid or 10% ethanol aqueous solution, respectively (Ashby, Cooper, Shorten, & Tice, 1992; Garde, Catala, & Gavara, 1998; Lickly, Markham, & McDonald, 1993). However, fatty food simulants are not such good substitutes of fatty foodstuffs. Oils probably yield mass transfer data very similar to those occurring in real fatty food/package systems, but analysis is very complicated, due to the numerous oil components and their non-volatility. Instead, other pure liquids are used, which vary considerably in chemical nature, ranging from non-polar *n*-heptane or *i*-octane to polar *i*-propanol or ethanol (Piringer, Franz, Huber, Begley, & Mc Neal, 1998; Sarria-vidal, De-La-Montana-Miguelez, & Simal-Gandara, 1997).

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In general, partition coefficient is defined as the ratio migrant equilibrium concentration in the food simulant $C_s$, to its equilibrium concentration in the gas phase $C_g$:

$$K = \frac{C_s}{C_g} \tag{1}$$

There are other methods for calculation of partition coefficients. Two methods were performed: the "vapour phase calibration" method (VPC) (Kolb, Welter, & Bichler, 1992), and the "phase ratio variation" method (PRV) (Ettre, Welter, & Kolb, 1993).

The VPC method was described for the determination of the partition coefficient of a compound in a gas–liquid using GC–HS. In this method, the compound equilibrium concentration in the liquid phase present in the headspace vial is calculated as the difference.

There is another possibility for establishing the partition coefficient of a compound in a gas–liquid system from GC–HS. This method is based on the relationship between the partition coefficient and the phase ratio.

Our objectives were to determine the partition coefficient of six solvents in food simulant/air system by the PRV method and to investigate the influence of the food structure on the absorption of solvents.

## 2. Materials and methods

### 2.1. Phase ratio variation (PRV method)

The original sample solution is defined by $V_S$, $m_S$ and $C_{in}$.

$V_S$ = volume of the original sample solution introduced into the sample vial, $m_S$ = the mass of the volatile compound in the original sample and $C_{in}$ = the initial concentration of the volatile compound in the original sample expressed as mass per volume:

$$C_{in} = \frac{m_S}{V_S} \tag{2}$$

The phase ratio ($\beta$) of the vial is the ratio of the volumes of the headspace ($V_G$) and the sample solution ($V_S$):

$$\beta = \frac{V_G}{V_S} \tag{3}$$

Generally the volume of the gas phase (headspace) is taken as the difference between the volumes of the sample vial ($V_V$) and the sample solution ($V_S$):

$$V_G = V_V - V_S \tag{4}$$

Partition coefficient is defined as the ratio of migrant (volatile compound or solvent) equilibrium concentration in the solution material, $C_S^*$, to its equilibrium concentration, in the gas phase, $C_G^*$.

$$K = \frac{C_S^*}{C_G^*} \tag{5}$$

Defining the tow concentration as:

$$C_S^* = \frac{m_S^*}{V_S} \tag{6}$$

$$C_G^* = \frac{m_G^*}{V_G} \tag{7}$$

the partition coefficient can be expressed as:

$$K = \frac{C_S^*}{C_G^*} = \frac{m_S^*}{m_G^*} \cdot \frac{V_G}{V_S} = \frac{m_S^*}{m_G^*} \cdot \beta \tag{8}$$

$m_S$ is defined as:

$$m_S = m_S^* + m_G^* \tag{9}$$

$$\frac{m_S}{V_S} = \frac{m_S^*}{V_S} + \frac{m_G^*}{V_S} \tag{10}$$

but $V_S = \frac{V_G}{\beta}$; therefore,

$$\frac{m_S}{V_S} = \frac{m_S^*}{V_S} + \frac{m_G^*}{V_G} \cdot \beta \tag{11}$$

$$C_{in} = C_S^* + C_G^* \cdot \beta \tag{12}$$

$$C_S^* = K \cdot C_G^*; \tag{13}$$

therefore,

$$C_{in} = K \cdot C_G^* + C_G^* \cdot \beta = C_G^*[K + \beta] \tag{14}$$

and thus,

$$C_G^* = \frac{C_{in}}{K + \beta} \tag{15}$$

Taking reciprocals of both sides of Eq. (15) we obtain:

$$\frac{1}{C_G^*} = \frac{K}{C_{in}} + \frac{1}{C_{in}} \cdot \beta \tag{16}$$

However, in headspace analysis, the peak area ($A$) is proportional to the equilibrium concentration in the headspace of the vials:

$$A = f_i \cdot C_G^* \tag{17}$$

$$C_G^* = \frac{A}{f_i} \tag{18}$$

Therefore, in order to establish the value of $C_G^*$, one would need the value of $f_i$, which is a proportional factor, depending also on the particular system and the analytical conditions. However, there is an easy way to overcome this problem. Substituting $\frac{A}{f_i}$ for $C_G^*$ into Eq. (16):

$$\frac{f_i}{A} = \frac{K}{C_{in}} + \frac{1}{C_{in}} \cdot \beta \tag{19}$$

$$\frac{1}{A} = \frac{K}{f_i} \cdot \frac{1}{C_{in}} + \frac{1}{f_i} \cdot \frac{1}{C_{in}} \cdot \beta \tag{20}$$

$$\frac{1}{A} = a + b \cdot \beta \tag{21}$$

where

$$a = \frac{K}{f_i \cdot C_{in}} \tag{22}$$

$$b = \frac{1}{f_i \cdot C_{in}} \tag{23}$$

and

$$K = \frac{a}{b} \tag{24}$$

In other words, we can plot $\frac{1}{A}$ against $\beta$ and carry out regression analysis of this plot, establishing its slope ($b$) and intercept ($a$).

### 2.2. Instrumentation

The measurements were made on a Perichrom Sarl model PR 2100 automatic Headspace Sampler on the Gas Chromatograph (with flame-ionization detector). The volume of the headspace vial = 11 ml.

A fused silica capillary column (Varian, Canada) was employed (length 30 m:WCOT Fused silica 30 m × 0.25 mm, Coating: CP WAX 52CB DF = 0.25UM). The conditions for gas chromatography were as follows: oven temperature programme: 100 °C. The carrier gas was nitrogen at a flow rate of 229 ml/min.

Detector and injector temperatures were 260 and 250, respectively. Air, $H_2$ and $O_2$ flow rates were 18, 50, 50 ml/min, respectively. Carrier injector 100/100, split 40/40.

### 2.3. Sample preparation

Aqueous solutions of food simulants (Water distilled, 3% acetic acid, 10% ethanol, 95% ethanol) were prepared with 10 μl pure migrant (acetaldehyde, acetonitrile, butyraldehyde, ethyl acetate, ethyl methyl ketone, isopropyl acetate) introduced to 100 ml of each food simulant (Fig. 2). Some properties of these solvents are shown in Table 1. The molecular descriptors for each compound were calculated from knowledge of the Molecular Modeling Pro. Version 5 (ChemSW Software Inc.) (Molecular Modeling Pro Version 5, 2002).

Table 1
Purity, company and molecular weights of solvents

| Solvents | Purity (%) | Company | Molecular weight | Polarity[a] |
|---|---|---|---|---|
| Acetonitrile | >99 | CARLO ERBA (France) | 41.05 | 18.03 |
| Acetaldehyde | 99% | MinMERCK (Germany) | 44.05 | 8.00 |
| Ethanol | 99.% | PROLABO (France) | 46.06 | 8.80 |
| Acetic acid | 99.5% | MERCK (Germany) | 60.05 | 7.91 |
| Butyraldehyde | 99% | PROLABO (France) | 72.10 | 5.27 |
| Methyl ethyl ketone | >99% | Fisher Scientific (UK) | 72.10 | 9.01 |
| Ethyl acetate | >99.7% | MERCK (Germany) | 88.10 | 5.35 |
| Iso-propyl acetate | >99 | MERCK (Germany) | 102.13 | 4.14 |

[a] Data from the software of Molecular Modeling Pro (2002).

Increasing volumes (1, 2, 3, 4 and 5 ml) of this solution were placed into headspace vials (11 ml) and sealed with magnetic septa (perichrom); thus, each vial represented a gas/liquid phase ratio, $\beta$, of 10; 4.5; 2.67; 1.75; 1.2, respectively, calculated according to Eq. (3).

Equilibrium times for each solvent at 20 °C were determined by plotting % differences between controls and sample headspace values until they did not change. After storing each vial for 1 day (equilibrium day according to solvent and sample), a 1 ml sample of headspace was injected into the GC by gas tight syringe.

## 3. Results and discussion

### 3.1. Partition coefficients of six migrants

The partition coefficients of the six migrants were determined in four food simulants at 20 °C. For each food simulant, the gas phase in each vial was analyzed from vials with different phase ratios. Linear regression analysis was performed according to Eq. (21) where $x = \beta$ and $y = 1/A$. The partition coefficient ($K$) was calculated using Eq. (24). The *food simulant/air* partition coefficients of migrants were calculated according to the PRV (phase ratio variation) method. Table 2 shows the chromatography peak area for each gas phase, the results of linear regression analysis and the calculated partition coefficient values for the ethyl acetate in four food simulants.

According to Table 2, partition coefficients of ethyl acetate between water, 10% ethanol, 3% acetic acid food simulants and air ranged from 34 to 39. The highest partition coefficient of ethyl acetate, obtained with 95% ethanol, was 140.

EA was thus found to be highly soluble in 95% ethanol and less in the other food simulants. Peak areas were the average ± standard deviation of 15 assays on each volume (for each sample). Table 3 shows the physicochemical properties of EA and the food simulants.

From Table 2, it can be concluded that ethyl acetate is hydrophobic. There was a linear relationship between the Log $P$ value and the partition coefficient. The octanol/water partition coefficient (Log $P$) is the standard quantity for characterizing the hydrophobicity/hydrophilicity of a molecule (Katritzky, Lobanov, & Karelson, 1997). Log $P$ is linked to the hydrophobicity of a migrant. The higher the Log $P$, the more hydrophobic is the compound. Another reason for the high partition coefficient of EA in 95% ethanol was the solubility parameter. The total solubility parameter, $\delta$ (Hansen solubility), was the sum of three parts, corresponding to a nonpolar interaction $\delta_d$, polar interaction $\delta_p$, and hydrogen-bonding interaction, $\delta_h$ (Hansen, 1967).

Moreover, the heat of mixing was estimated from properties of the pure substances. The smaller the difference between the $\delta$ values of two substances, the greater was the solubility. For this reason, the term $\delta$ has been pro-

Table 2
Data for ethyl acetate, in four food simulants

| Name of the solutions | Volume of solution in vial (ml) | Phase ratio ($\beta$) | Peak area (A) | Linear regression analysis | | | Partition coefficient ($K_{F/air}$) |
|---|---|---|---|---|---|---|---|
| | | | | Slop ($b'$) | Intercept ($a'$) | Correlation coefficient ($R^2$) | |
| Water | 1 | 10 | 53.07 ± 1.44 | 0.0003983 | 0.0150150 | 0.96810 | 37.7 ± 0.7 |
| | 2 | 4.5 | 58.20 ± 1.55 | | | | |
| | 3 | 2.67 | 61.56 ± 1.16 | | | | |
| | 4 | 1.75 | 64.48 ± 1.28 | | | | |
| | 5 | 1.2 | 65.31 ± 1.65 | | | | |
| Ethanol 10% | 1 | 10 | 50.50 ± 0.80 | 0.0004068 | 0.0157573 | 0.99902 | 38.7 ± 0.1 |
| | 2 | 4.5 | 56.72 ± 0.79 | | | | |
| | 3 | 2.67 | 59.18 ± 0.77 | | | | |
| | 4 | 1.75 | 60.81 ± 2.10 | | | | |
| | 5 | 1.2 | 61.74 ± 1.08 | | | | |
| Acetic acid 3% | 1 | 10 | 46.03 ± 1.72 | 0.0004892 | 0.0169089 | 0.98853 | 34.6 ± 0.4 |
| | 2 | 4.5 | 52.07 ± 2.18 | | | | |
| | 3 | 2.67 | 54.17 ± 0.49 | | | | |
| | 4 | 1.75 | 56.31 ± 2.14 | | | | |
| | 5 | 1.2 | 58.01 ± 0.39 | | | | |
| Ethanol 95% | 1 | 10 | 11.37 ± 0.11 | 0.0005851 | 0.0822751 | 0.97554 | 140.6 ± 0.6 |
| | 2 | 4.5 | 11.70 ± 0.30 | | | | |
| | 3 | 2.67 | 11.96 ± 0.21 | | | | |
| | 4 | 1.75 | 12.00 ± 0.38 | | | | |
| | 5 | 1.2 | 12.08 ± 0.08 | | | | |

Table 3
Physicochemical properties of migrants and solutions

| Name of migrant and solution | Molecular weight[a] | Log $P$[a] | Solubility in water ($\delta$)[a] |
|---|---|---|---|
| Acetonitrile | 41.05 | −0.39 | 24.42 |
| Acetaldehyde | 44.05 | −0.22 | 20.19 |
| Butyraldehyde | 72.10 | 0.83 | 17.10 |
| Methyl ethyl ketone | 72.10 | 0.26 | 18.97 |
| Ethyl acetate | 88.10 | 0.67 | 18.13 |
| Iso-propyl acetate | 102.13 | 1.20 | 17.48 |
| Ethanol 95% | 44.66 | −0.28 | 27.55 |
| Ethanol 10% | 20.82 | −1.05 | 45.66 |
| Acetic acid 3% | 19.27 | −1.12 | 47.00 |
| Water | 18.01 | −1.15 | 47.80 |

[a] Data from the software of Molecular Modeling Pro (2002).

posed as the solubility parameter (Nielsen, Margaretha-Jägerstad, Öste, & Wesslén, 1992).

Consequently, a comparison of the $\delta$ values of a food simulant and migrant gave an indication of the solubility.

### 3.2. Partition coefficient of other migrants between food simulants and air

Table 4 shows the partition coefficients of five migrants in a food stimulant/air system.

$K$ was calculated from the values of $a$ and $b$ obtained by plotting $1/A$ against $\beta$.

According to Eqs. (20) and (21):

$$\frac{1}{A} = a + b \cdot \beta \tag{21}$$

where

$$a = \frac{K}{f_i \cdot C_{in}} \tag{22}$$

$$b = \frac{1}{f_i \cdot C_{in}} \tag{23}$$

then

$$K = \frac{a}{b} \tag{24}$$

Table 4 presents the partition coefficient of methyl ethyl ketone (2-butanone) (Fig. 1) between four simulants and air. $K$ values for systems containing water, 10% ethanol and 3% acetic acid as food simulants were in the range 34–36. For 95% ethanol, the partition coefficient increased up to 57. This result was expected since ethanol and methyl ethyl ketone (MEK) have very similar chemical structures.

Table 3 shows physicochemical characteristics of MEK and food simulants.

Affinity of MEK for 95% ethanol shows a common feature with EA. These results indicate that migrant polarity was the predominant controlling factor and that a simulant with similar high polarity had a great effect on sorption. Partitioning depends on the polarity and solubility of migrant in the food stimulant (Le-Thanh, Thibeaudeau, Thibaut, & Voilley, 1992; Nielsen et al., 1992).The difference between the values of 95% ethanol and MEK is 7.52 while for water and MEK, it is 28.8. Therefore, $\Delta\delta$ (difference of solubility parameters) increased as partition coefficient decreased.

Partition coefficient of iso-propyl acetate (IP) in *food simulants/air* is given by $K$ values in water, 10% ethanol,

Table 4
Partition coefficients of five migrants between food simulants and air

| Name of the migrant | Name of the solution | Linear regression analysis | | | Partition coefficient ($K_{F/air}$) |
|---|---|---|---|---|---|
| | | Slope ($b$) | Intercept ($a$) | Correlation coefficient | |
| MEK | Water | 0.0006570 | 0.0228705 | 0.98860 | 34.8 ± 0.4 |
| MEK | 10% Ethanol | 0.0007451 | 0.0259658 | 0.98065 | 34.8 ± 0.5 |
| MEK | 3% Acetic acid | 0.0006251 | 0.0223930 | 0.95367 | 35.8 ± 0.8 |
| MEK | 95% Ethanol | 0.0014840 | 0.0851859 | 0.95495 | 57.4 ± 0.8 |
| IP | Water | 0.0001594 | 0.0065509 | 0.91766 | 41.1 ± 1.1 |
| IP | 10% Ethanol | 0.0002147 | 0.0086710 | 0.98552 | 40.4 ± 0.4 |
| IP | 3% Acetic acid | 0.0001824 | 0.0070172 | 0.99781 | 38.5 ± 0.2 |
| IP | 95% Ethanol | 0.0022527 | 0.1069049 | 0.96714 | 47.5 ± 0.7 |
| BA | Water | 0.0004276 | 0.0174997 | 0.89136 | 40.9 ± 1.2 |
| BA | 10% Ethanol | 0.0004059 | 0.0206378 | 0.88163 | 50.8 ± 1.1 |
| BA | 3% Acetic acid | 0.0004739 | 0.0142613 | 0.96450 | 30.1 ± 0.7 |
| BA | 95% Ethanol | 0.0244503 | 0.1634857 | 0.98501 | 6.7 ± 0.4 |
| AA | Water | 0.0014523 | 0.0580058 | 0.98132 | 39.9 ± 0.5 |
| AA | 10% Ethanol | 0.0012279 | 0.0424414 | 0.96335 | 34.6 ± 0.7 |
| AA | 3% Acetic acid | 0.0011876 | 0.0430460 | 0.97064 | 36.2 ± 0.6 |
| AN | Water | 0.0015804 | 0.0669678 | 0.98126 | 42.4 ± 0.5 |
| AN | 10% Ethanol | 0.0011269 | 0.0523069 | 0.91067 | 46.4 ± 0.1 |
| AN | 3% Acetic acid | 0.0014846 | 0.0726763 | 0.91279 | 48.9 ± 1.1 |

MEK: Methyl ethyl ketone; IP: Iso-propyl acetate; BA: Butyraldehyde; AA: Acetaldehyde; AN: Acetonitrile.

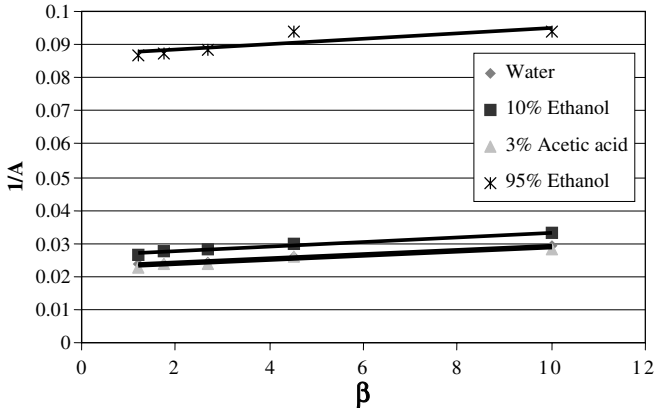


Fig. 1. Partition coefficient of methyl ethyl ketone between four food simulants and air.

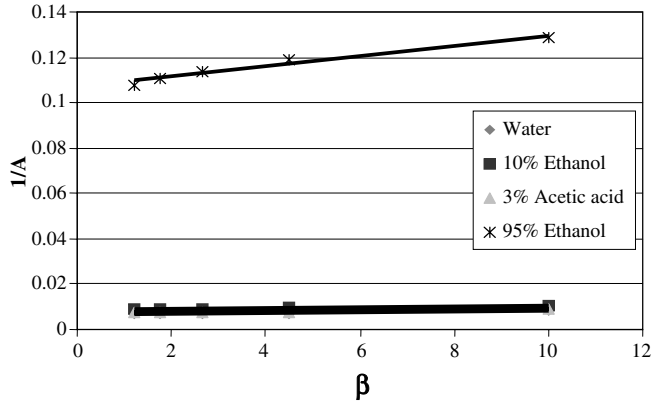


Fig. 2. Partition coefficient of isopropyl acetate between four food simulants and air.

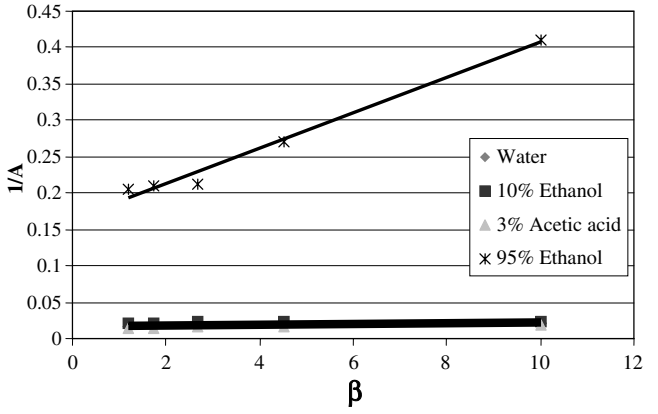


Fig. 3. Partition coefficient of butyraldehyde between four food simulants and air.

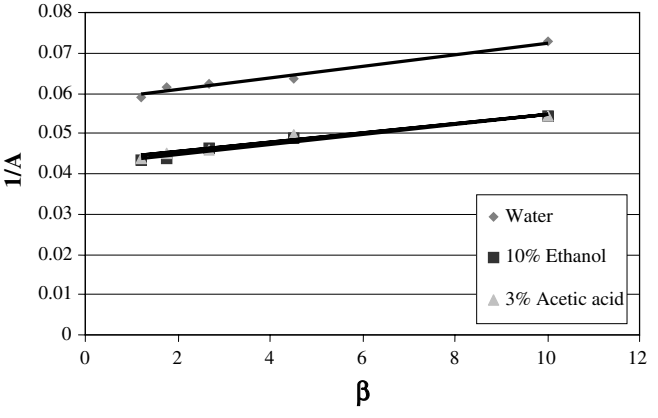


Fig. 4. Partition coefficient of acetaldehyde between four food simulants and air.

3% acetic acid and 95% ethanol, which were between 38 and 48 (Fig. 2).

As seen from results there were no major differences between amounts of migrant absorbed by the four food simulants. This phenomenon resulted from a reduction in the polar character of IP. When the carbon chain length increases, Log *P* increases (Jouquand, Ducruet, & Giampaoli, 2004). This is explained by the fact that IP did not have a high affinity for the four food simulants. Nevertheless, 95% ethanol absorbed larger amounts of IP than did the three simulants. The reason for this is the solubility parameter of 95% ethanol shown in Table 3, which is close to that of IP.

The difference between the esters might be linked to the length of the carbon chain, the longer the chain, the less polar is the ester. The compounds were easily absorbed by the non polar solutions. The solubility parameter of EA is higher in 95% ethanol than IP. For this reason, EA was more absorbed than was IP in 95% ethanol.

Partition coefficients of butyraldehyde (BA) were in the range of 30–51 for water, 10% ethanol and 3% acetic acid. For 95% ethanol, this value decreased to 6.68 (Fig. 3).

Knowledge of the binding behaviour of migrant to food components and their partitioning between different phase is of great importance in estimating the rate and amount of absorption by food simulnat. The partition coefficients of different classes of migrants depend largely on their polarity and solubility. In the case of water, 10% ethanol and 3% acetic acid, the solubility parameters of the solutions and BA are very close. Despite the fact that the solubility of BA and 95% ethanol solution are close, the partition coefficient is poor. The reason for this is unclear, but may be a consequence of the saturation of food simulant by BA that influenced the partition coefficient.

The partition coefficient of acetaldehyde (AA) is shown in Table 4. *K* values of AA in three simulants were between 34 and 39 (Fig. 4). From the results in this table, there were no major differences between the three partition coefficients. The solubility parameter and hydrogen-bonding influenced the partition coefficient. Unfortunately, for 95% ethanol, we could not identify surface area (*A*) of AA, because *A* of 95% ethanol was very wide.

Comparison between acetaldehyde and butyraldehyde showed that the absorption of a series of compounds with the same functional group increased with an increasing number of carbon atoms in the molecular chain, up to a certain limit (Fukamachi, Matsui, Hwang, Shimoda, & Osajima, 1996; Landy, Druaux, & Voilley, 1995).

Partition coefficients of acetonitrile (AN) in three food simulants were in the range 42–49 (Fig. 5). The effects of polarity, solubility and hydrogen-bonding character were also observed by comparing the absorption behaviour in the food simulants. In addition, the N atom in acetonitrile increased the hydrogen-bonding character of this molecule. For the same reason as for AA, we did not identify the surface area of AN in head space.

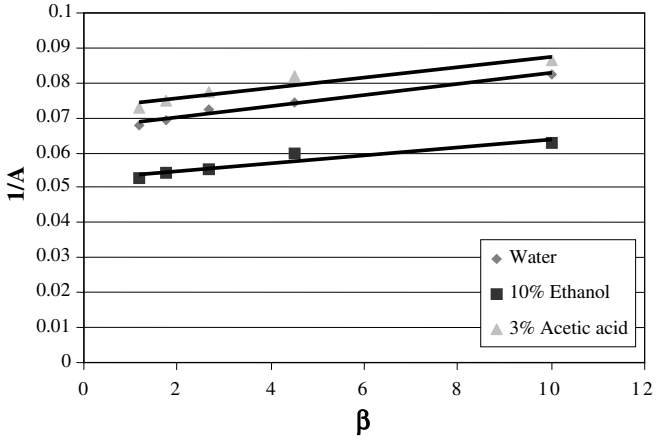


Fig. 5. Partition coefficient of acetonitrile between four food simulants and air.

## 4. Conclusion

Partition coefficients of six migrants were determined between four food simulants and air by the phase ratio variation methods using headspace chromatography. It should be emphasized that the gas–liquid partition coefficient values estimated by the PRV method described in this paper are useful data for *K* values in gas chromatography.

The amount of migrants absorbed into different food simulants depends partly on the nature of the food and partly on the chemical features of the migrant. Factors that affected absorption include molecular size of migrants, and polarity and solubility properties of both the food simulants and the migrants.

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