

ANALYSIS OF MIXTURES OF ORGANIC VOLATILE COMPOUND IN WATER BY MIMS. SEMIQUANTITATIVE EVALUATION OF DATA

Natálie MUSILOVÁ-KEBRLOVÁ^{a,*} and Pavel JANDERKA^b

^a *Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, v.v.i, 162 06 Prague 6, Czech Republic; e-mail: musilovan@centrum.cz*

^b *Pragolab s.r.o., Jamborova 25, 61500, Brno, Czech Republic; e-mail: janderka@pragolab.cz*

Received November 17, 2008

Accepted February 19, 2009

Published online March 30, 2009

Chemometric analysis of intensities of ion currents measured by MIMS was demonstrated on two mixtures: nonpolar mixture containing benzene–toluene–*p*-xylene (set I) and polar mixture containing methanol–ethanol–propan-1-ol (set II), both in water solutions. The acquired MIMS data were evaluated off-line using Solver, a tool of Microsoft Excel and then verified by calculation of relative concentrations of components in mixtures. For evaluation we considered the additivity of ion currents coming from fragmentation of components, independent vapor permeation of components through membrane and unimolecular conditions in ion source of MS. By using this evaluation analysis it is possible to determine relative concentrations of organic substances in mixture, which penetrated through the membrane, without any separation. Set I penetrated according to the model analysis and the obtained relative concentrations were in reasonable agreement with the preset values. On the contrary, for set II the agreement of adjusted and calculated relative concentrations was not achieved due to high dielectric permittivity of alcohols.

Keywords: Membrane introduction mass spectrometry; MIMS; Direct inlet probe; DIP; Volatile organic compounds; VOC; Mixture analysis; Chemometrics.

Membrane introduction mass spectrometry (MIMS) has achieved status of a particularly selective and sensitive method in analysis of low-concentrated volatile organic species in gases and liquids^{1–7} including the environmental samples^{5,6,8–12} in water solutions. MIMS technique were used for monitoring of some processes in chemical, electrochemical^{13,14}, biochemical¹⁵ and photochemical reactions³.

MIMS enables direct connection of mass spectrometer with solution, which is separated from vacuum space of MS by hydrophobic, semi-permeable membrane (typically silicone polymer, PTFE, PVDF, or polypropylene)^{2,13}. The membrane behaves as a separator, which enables selective input of a compound from solution into the MS. Its capability of

separation depends not only on the instrumental factors such as thickness, material, pore size and porosity of membrane but also on the polarity and volatility of compounds.

MIMS spectra of a mixture usually contain overlapping fragments of m/z . This is due to the fact that individual compounds of a mixture contain in their spectra certain fragments of m/z which are also present in spectra of other compounds (e.g., m/z 49 is present in spectra of benzene and *p*-xylene). Therefore, it is very difficult to determine the percentage of the ion intensity for m/z coming from one of the compounds.

Due to the problematic interpretation of MIMS spectra we invented an off-line multicomponent analysis (further referred to as "analysis"). The main goal of the analysis was obtaining the information about relative concentration of compounds in mixture without absolute calibration of MS and determination of the relative population of particular compounds in the reaction mixture.

Therefore, we analyzed specific chosen ion currents I_i (characteristic of given compound) using Solver (in MS Excel, Microsoft). The analysis was based on the assumption that the mass spectrometrically determined ion intensity I_i is directly proportional to the molar concentrations in solution, c_i (partial pressure p_i) of that species¹³ i

$$I_i = ac_i = bp_i = K^0 J_i \quad (1)$$

where a , b and K^0 are constants of proportionality and $J_i = dn/dt$ is the input flow of compound in mol s^{-1} .

The flow of substances through the membrane in the steady state^{1,13,16} is described by Fick's equation of diffusion

$$J = \frac{A}{L} D c \frac{s_m}{s_w} \times 10^{-3} \quad (2)$$

where J is flow of a substance (mol s^{-1}), A is the surface of membrane (cm^2), L is the thickness of the membrane (cm), D is diffusion coefficient ($\text{cm}^2 \text{s}^{-1}$), c is the concentration of analyte in solution (mol l^{-1}) and s_m and s_w are solubility of substance in membrane and water (mol l^{-1})¹⁶, respectively.

The constant K^0 can be calculated from the pressure decrease in the calibration volume V_c , i.e. from a plot of the ion current I_i versus the differentiated pressure p_c ¹³

$$I_i = (K^0 / RT) V_c dp_c / dt. \quad (3)$$

Previously we investigated redox, adsorption and desorption processes on electrode^{17–19} using membrane input combined with electrochemical cell (differential electrochemical mass spectrometry (DEMS)). In DEMS, products of electrochemical reaction pervaporated from the electrochemical cell through the membrane to MS and a mixture of spectra of many fragments m/z is obtained. Sometimes it is difficult to assign fragments of m/z to intermediates and products of dynamic process and to determine relative population of intermediates and products in the reaction mixture. So, another aim of the analysis of MS data is to confirm or exclude the hypothesis of the presence or absence of expected products and intermediates in dynamic systems.

Experimental

General

General scheme of the experimental set-up showing the design of chemical cell and its connection to the mass spectrometer was described in previous papers^{13,14}.

The used mass spectrometer was a quadrupole Trio 1000 (Finnigan MAT, Fisons Instruments, San José, California, USA): mass range m/z 2–1000, temperature in the ion source 150 °C, EI ionization mode at 70 eV and electron multiplier as a detector. The mass spectrometer response is expressed in arbitrary units, proportional to the ion current of specific m/z values. For all measurements we used the single ion monitoring mode (SIM mode), which facilitates more sensitive measurement of selected ions. For individual spectrum of benzene we followed 23 masses, for toluene 20 and for *p*-xylene 21 masses and for set I totally 24 masses. For methanol 7 masses were followed, for ethanol 17 masses and for propan-1-ol 19 masses. For set II 13 masses were observed.

The vacuum connection of membrane interface with the ion source of the mass spectrometer was provided by the manual control vacuum valve (Balzers, type EVA 016 HX) and by the sample probe inlet valve, using the home-made stainless construction. Vapor pressure below the membrane was measured by temperature-compensated compact capacitance gauge CMR 263 (Pfeiffer Vacuum) with measuring range 10^{-3} –11 mbar. In the case of standard PTFE membrane the typical value of vapor pressure in ionization chamber was 9 Pa (ca. 7×10^{-2} Torr). The real pressure was higher than 1.33×10^{-5} Pa (10^{-7} mTorr). Under these conditions the ion/molecules reactions in ion source are negligible.

The used membrane was made of PTFE (GoreTex, No. S10570, pore 0.02 μm , thickness 75 μm , porosity 50%). The critical size of membrane pores was estimated at $r < 0.8 \mu\text{m}$ (external pressure 1 bar, the pressure on the opposite side of membrane 1×10^{-2} Pa, surface tension²⁰ $\sigma = 72 \times 10^{-5} \text{ N cm}^{-1}$ and contact angle²¹ $\Theta = 120^\circ$). The membrane active area was determined by the exposed area 0.785 cm^2 of supporting porous steel frit Siper® R14 (Tridelta Siper GmbH, Dortmund, Germany) with average pore size 14 μm and porosity² 26%. During the measurements, constant temperature was maintained.

Water solutions of mixtures were prepared by mixing the same volumes of stock solutions of pure substances directly in MIMS cell (1:1:1 v/v/v). The ratio of pure component concen-

trations in set I was kept at the experimental ratio 1:0.84:0.74 (benzene-toluene-*p*-xylene) and in set II at the experimental ratio 1:0.69:0.48 (methanol-ethanol-propan-1-ol).

Chemicals

For preparation of solutions, Millipore water (18.2 MΩ purification system, Milli-Q RG), methanol, ethanol, propan-1-ol, benzene, toluene and *p*-xylene were used, all of analytical grade. Some of the physical properties of pure compounds are compiled in Table I.

RESULTS AND DISCUSSION

Theory

The assumptions for a multicomponent system are the following: (i) negligible interaction of components during vapor permeation through the membrane, (ii) negligible interaction of components in the ion source of MS and (iii) additivity of ion currents I_i coming from fragmentation of the present components. Conditions for fulfilling these requirements are similar features of the compounds such as structure, volatility and polarity.

The relationship between the ion current of the i -th m/z value for the j -th substance I_{ij} and the amount of substance in analyte is equal to

$$I_{ij} = a p_j = K^0 J_j \quad (4)$$

and the relationship for the substance flow through the membrane (provided that the assumptions (i) and (ii) are met) is

TABLE I
Selected physicochemical properties of the compounds¹⁶ used

Compound	M_w^a	T_b^b	μ^c	ε^d	γ^e	c_w^f	$\log P_{ow}^g$
Methanol	32.04	64.6	5.67	32.70	22.07	miscible	-0.74
Ethanol	46.07	78.29	5.54	24.55	21.97	miscible	-0.3
Propan-1-ol	60.10	97.2	5.60	20.33	23.32	miscible	0.25
Benzene	78.11	80.09	0	2.275	28.22	1.78	2.13
Toluene	92.14	110.63	1.2	2.379	27.93	0.515	2.73
<i>p</i> -Xylene	106.17	138.3	0	2.270	28.01	0.215	3.15

^a Molar mass (g mol⁻¹); ^b normal boiling points (°C); ^c dipole moment (D); ^d relative permittivity, ^e surface tension²⁶ (m N/m⁻¹), ^f solubility in water (g l⁻¹), ^g octanol-water partition coefficient.

$$J_j = \frac{A}{L} D c \frac{s_m}{s_w} = J'_j / RT \quad (5)$$

where p_j is the partial pressure of the j -th component, a a proportionality constant, J_j the input flux in mol s^{-1} , J'_j the flow of molecules through the membrane in $\text{mbar l s}^{-1} \text{ cm}^{-2}$ (the meaning of other symbols is the same as in Eqs (1) and (2)).

We assume that the dependence of I_{ij} on concentration is linear

$$I_{ij} = k_{ij} c_j a_{ij} \quad (6)$$

where c_j is the molar concentration of the j -th compound in solution, a_{ij} the relative intensity of ion current I_{ij} in the MIMS spectrum used as standard spectrum of the j -th pure substance (it characterizes the fragmentation of a given substance in ion source) and k_{ij} a proportionality constant.

For a mixture of compounds we presume the principle of additivity of ion currents (see (iii)) for the values of m/z

$$I_i = I_{i1} + I_{i2} + \dots + I_{ij} \quad (7)$$

The total ion current with respect to Eq. (6) is equal to

$$I_i = \sum_j k_{ij} c_j a_{ij} \quad (8)$$

where I_i is the additive ion current of the chosen m/z value originating from fragmentation of all present types of molecules.

For similar species, if we assume that $k_{i1} \cong k_{i2} \cong k_{ij} = k_p$, then Eq. (8) can be modified giving the following form

$$I_i = k_i \left(\sum_j c_j a_{ij} \right) \quad (9)$$

As proportionality constants k_i cannot be determined, only the ratio of concentration and its relative values $c_{j,\text{rel}}$ (with respect to the most concentrated component, e.g. benzene – set I and methanol – set II) can be calculated by using the modified Eq. (9) in the following form

$$I_{i,\text{rel}} = \sum_j c_{j,\text{rel}} a_{ij} \quad (10)$$

where $I_{i,\text{rel}}$ is the relative intensity of ion current of particular m/z in the MIMS spectrum of a mixture.

Equation (10) leads to the formation of a set of linear equations, one linear equation for each ion current of chosen m/z , with unknown relative concentrations $c_{j,\text{rel}}$ of components. Taking into account the inaccuracy of the experimental data the monitoring of $3N$ different ion currents of N species is recommended.

Set I: Aromatic Hydrocarbons

First we measured and evaluated the experimental mass spectra of pure compounds benzene, toluene and *p*-xylene (Fig. 1).

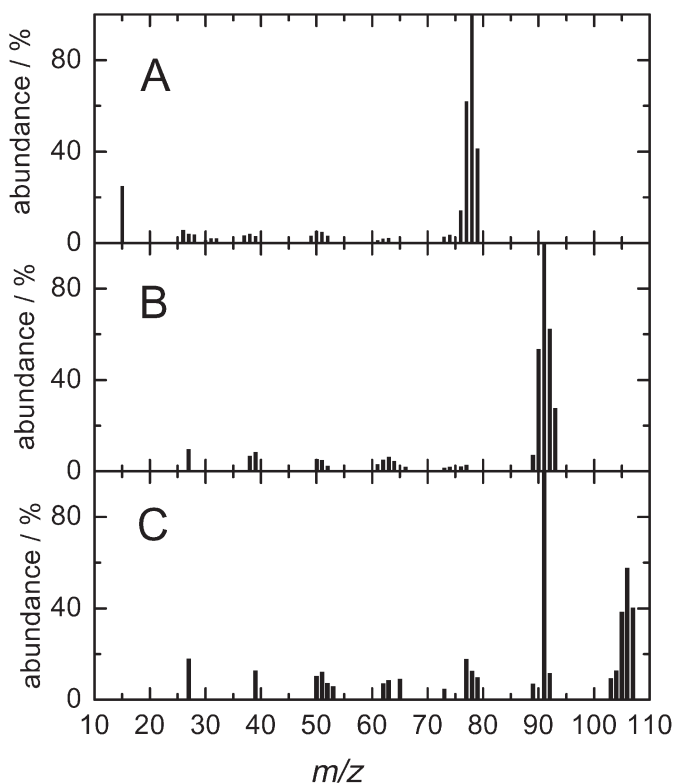


FIG. 1

MIMS spectra of benzene (A), toluene (B) and *p*-xylene (C) measured by water solution permeation through the Teflon membrane inlet at the highest concentrations (mol l^{-1}): 2.02×10^{-3} (A), 1.69×10^{-3} (B), 1.50×10^{-3} (C)

Vapor permeation of pure compounds through the membrane causes an increase in total ion current (TIC), in dependence on the volume of additions of pure compounds to water in MIMS cell (Fig. 2). We found 24 concentration-dependent ion currents in total. From experimental MIMS profiles of benzene (Fig. 2A), toluene (Fig. 2B) and *p*-xylene (Fig. 2C) it can be seen that the steady-state vapor permeation is reached in the case of benzene and toluene (within an experimental error), but only at lower concentrations of *p*-xylene. This shows that benzene and toluene diffuses through the membrane more rapidly than *p*-xylene. As the molecular weight of aromatic components increases, the flux decreases. The largest

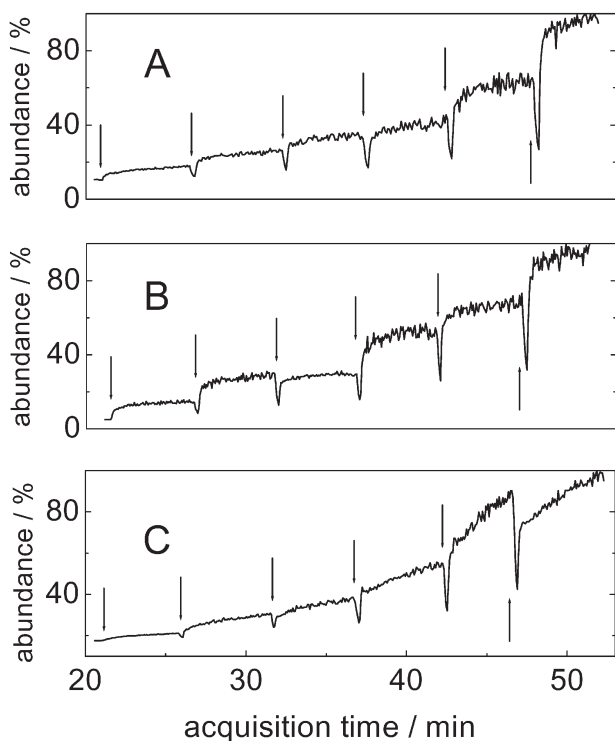


FIG. 2

MIMS profiles of concentration dependence of total ion currents (TIC) for pure benzene (A), toluene (B) and *p*-xylene (C) measured by gradual increasing concentrations of solution penetrating through the Teflon membrane inlet. The concentrations (mol l^{-1}): 2.24×10^{-4} – 2.02×10^{-3} (A), 1.88×10^{-4} – 1.69×10^{-3} (B), 1.67×10^{-4} – 1.49×10^{-3} (C). Arrows indicate the additions of standard solution

p-xylene molecule shows a low diffusion coefficient and low solubility in the membrane, which results in a decrease in its flux. On the other hand, the smaller benzene molecule shows a high diffusion coefficient and greater solubility in the membrane, which produces a higher flux. In order to eliminate differences in diffusivity and fluxes of components in the membrane, the concentration-dependent values of ion currents (TIC and single ion currents) were read at the end of a 5 min period after each addition.

Selection of characteristic values of m/z was verified by construction of calibration dependences for all pure substances; the TIC and most intensive ion currents are shown (Fig. 3A for benzene, Fig. 3B for toluene and Fig. 3C for *p*-xylene).

Then we measured and evaluated the experimental mass spectra of set I (benzene–toluene–*p*-xylene). The linear dependence of ion currents I_{26} , I_{45} , I_{49} , I_{78} and I_{79} (Fig. 4) on increasing concentration of mixture is related to their pervaporation. It is evident that the substance flow through the membrane obeys Fick's equation (Eq. (2)). The membrane transmits molecules to ionic source linearly in dependence of their concentration in the mixture.

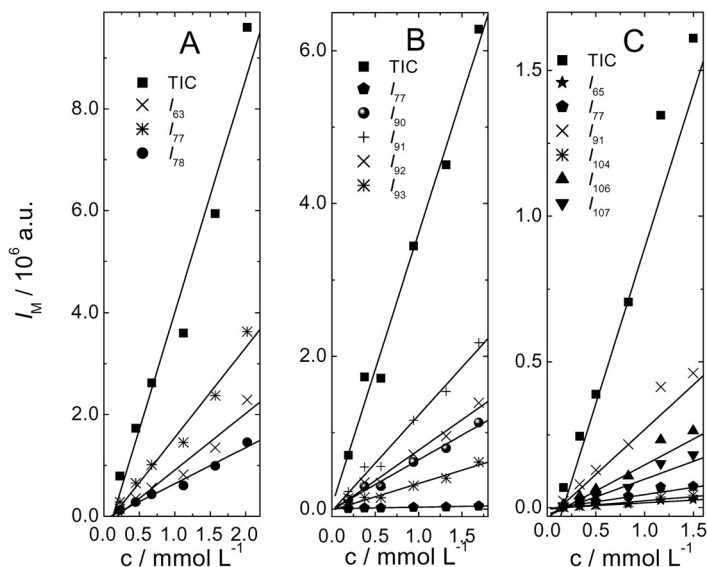


FIG. 3

Calibration dependence of total ion current (TIC) and individual characteristic ion currents I_M for benzene (A), toluene (B) and *p*-xylene (C)

The dependence of the ion current I_{26} (mass m/z 26 present only in benzene spectrum^{22,23}) on increasing concentration of benzene in set I was linear (Fig. 4A). The linearity of this dependence shows that pervaporation of benzene through the membrane is not affected by the presence of other substances in set I, i.e. toluene and *p*-xylene. Benzene penetrates independently through the membrane.

Concentration dependences of ion currents of masses m/z 49, 78 and 79 (Fig. 4B) present in spectra of benzene and *p*-xylene on increasing concentration of benzene and *p*-xylene in set I is also linear. Benzene and *p*-xylene contribute together to I_{49} , I_{78} and I_{79} in the measured spectra. We assume no contribution of toluene because m/z 49, 78 and 79 are not present in its characteristic spectrum.

Similarly, in Fig. 4C we can see the linear dependence of ion current I_{45} , ion current of toluene and *p*-xylene (fragment of m/z 45 is not present in mass spectrum of benzene) on the sum of concentrations of toluene and *p*-xylene in mixture.

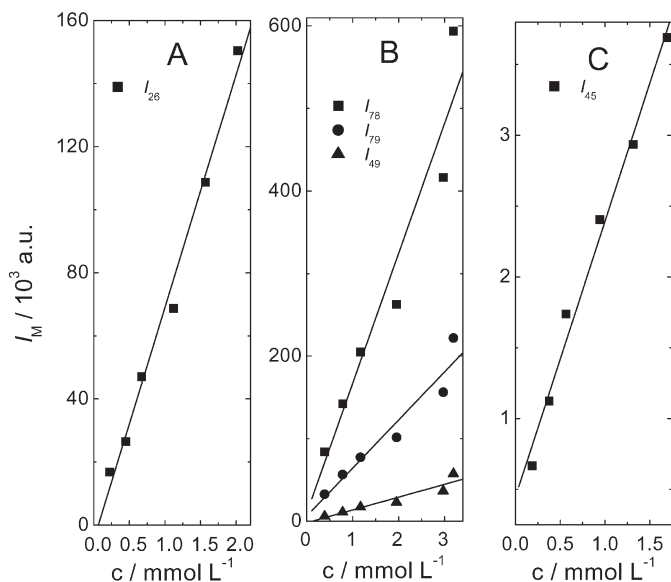


FIG. 4

Concentration dependences of selected ion currents I_M of m/z 26 on concentration of benzene in benzene–toluene–*p*-xylene (A), I_M of m/z 49, 78 and 79 coming from benzene and *p*-xylene on the sum of their concentrations (B), and I_M of m/z 45 coming from toluene and *p*-xylene on the sum of their concentrations (C), all in benzene–toluene–*p*-xylene (1:1:1 v/v/v)

The linear concentration relationship indicates that pervaporation of both substances through the membrane is independent and not affected by passing of a third substance (toluene Fig. 4B and benzene Fig. 4C).

Set II: Aliphatic Alcohols

First, similarly to set I, we measured and evaluated the experimental mass spectra of pure methanol, ethanol and propan-1-ol (Fig. 5). In total we found 27 concentration-dependent ion currents.

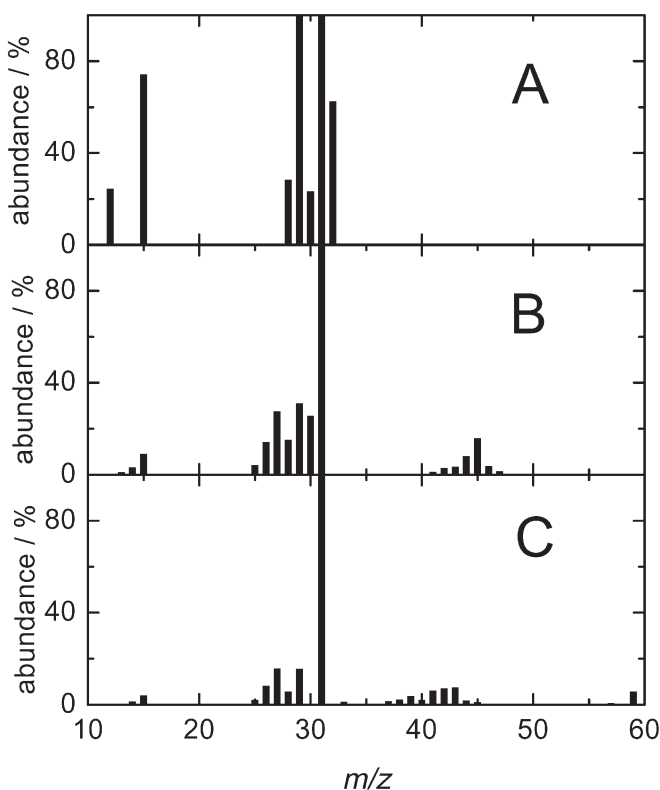


FIG. 5

MIMS spectra of methanol (A), ethanol (B) and propan-1-ol (C) measured by water solution permeation through the Teflon membrane inlet at the highest concentrations (mol l^{-1}): 3.94×10^{-2} (A), 2.70×10^{-2} (B), 1.87×10^{-2} (C)

Vapor permeation of pure components through the membrane causes an increase of total ion current (TIC), in dependence on the volume of additions of pure compounds to water in MIMS cell (Fig. 6).

From the MIMS profiles of pure components it can be seen that the time taken to reach the steady-state of vapor permeation decreases in the following order: propan-1-ol > ethanol > methanol. Johnson et al.²⁴ state that values of the diffusion coefficients D in silicone rubber membrane are $7.3 \times 10^{-11} \text{ m}^2 \text{ s}^{-1}$ for ethanol and $5.7 \times 10^{-11} \text{ m}^2 \text{ s}^{-1}$ for propan-1-ol²⁵ and in silicone capillary membrane are $4.2 \times 10^{-11} \text{ m}^2 \text{ s}^{-1}$ for methanol and $4.0 \times 10^{-11} \text{ m}^2 \text{ s}^{-1}$ for ethanol. It is clear that as the linear carbon chain of alcohol increases and their molecular weights increase, the diffusion coefficient decreases but the flux increases showing that the vapor permeation of long

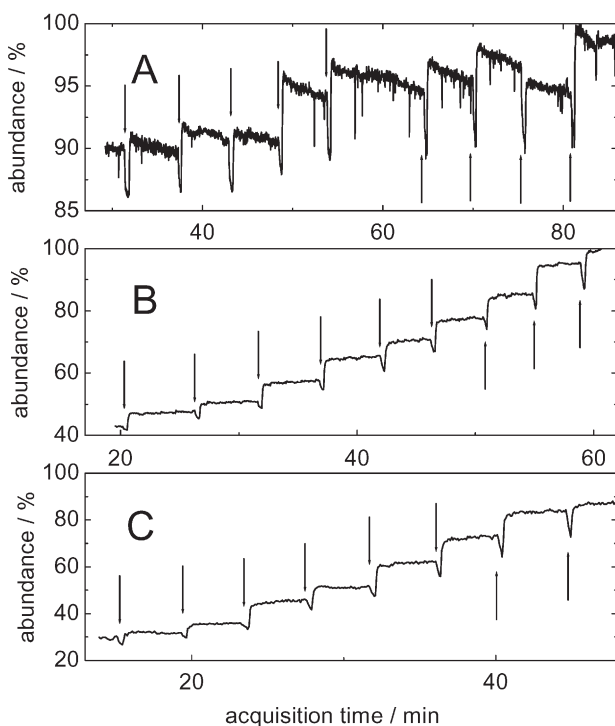


FIG. 6

MIMS profiles of concentration dependence of total ion currents (TIC) of methanol (A), ethanol (B) and propan-1-ol (C) measured by gradual increasing concentrations in the test water solutions through the Teflon membrane inlet. The concentrations (mol l^{-1}): 2.47×10^{-3} – 3.94×10^{-2} (A), 1.71×10^{-3} – 2.70×10^{-2} (B), 1.18×10^{-3} – 1.87×10^{-2} (C). Arrows indicate the additions of standard solution

carbon chains is favored. Alcohols of higher molecular weights show lower solubility in water and higher solubility in the membrane, which increases the flux. The reason why the steps on the MIMS profile of methanol are tilted can be the lowest solubility of methanol in nonpolar membrane due to the shortest carbonic chain and highest polarity in followed series of alcohols (Fig. 6A). The difference in solubility of the following alcohols illustrates the values of octanol-water partition coefficients in Table I.

For further measurements we chose 13 characteristic values of m/z ; their selection was verified by construction of calibration dependences for all pure substances. The TIC and most intensive ion currents are shown in Fig. 7.

Then we measured and evaluated the experimental mass spectra of set II (methanol-ethanol-propan-1-ol).

Figure 8A shows the linear concentration dependence of the ion current of mass m/z 30 (mass fragment for methanol and ethanol, absent in the propan-1-ol spectrum^{22,23}) on the sum of concentrations of methanol and ethanol in set II. Methanol and ethanol contribute together to the value of ion current of m/z 30 in the measured spectrum. We assume no contribu-

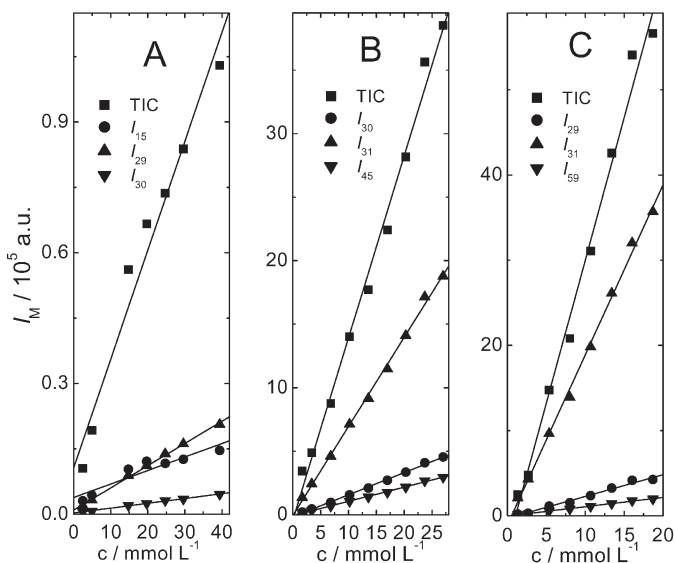


FIG. 7

Concentration dependence of total ion current (TIC) and selected individual ion currents I_M of methanol (A), ethanol (B) and propan-1-ol (C)

tion of propan-1-ol, because the m/z 30 is not present in its characteristic spectrum. The linear dependence of I_{30} indicates that vapor permeation of those substances through the membrane is linear, independent and not affected by passing of a third substance, i.e. of propan-1-ol. Nevertheless, the abundance of the mass m/z 30 in methanol spectrum amounts to one hundredth of the abundance in ethanol spectrum (not shown). So we assume the linear dependence of I_{30} in mixture is caused solely by ethanol vapor permeation.

Further, Fig. 8C shows a linear response of I_{46} (the unique fragment in MS of ethanol) to the concentration of ethanol in additions of set I. The linear dependence of I_{30} and I_{46} on increasing concentration of the mixture is related to pervaporation. It is evident that the flow of substance (ethanol) through the membrane is directed by Fick's equation (Eq. (1)). The membrane transmits molecules of ethanol to ionic source linearly in dependence on their concentration in solution – mixture.

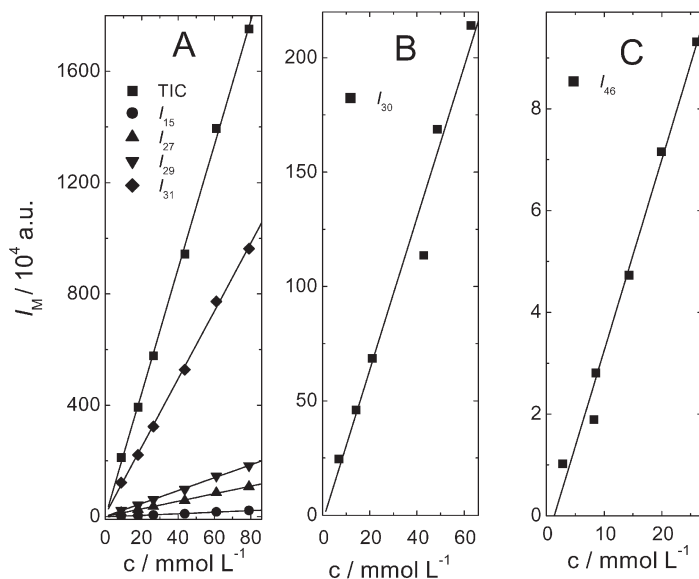


FIG. 8

Concentration dependences of selected ion currents I_M of m/z 15, 27, 29 and 31 (common ion currents for all components) on the sum of concentrations of methanol, ethanol and 1-propanol (A); I_M of m/z 30 (common ion current for methanol and ethanol) on the sum of concentrations of methanol and ethanol (B); and I_M of m/z 46 (unique ion current of ethanol) on concentration of ethanol (C); all in methanol–ethanol–propan-1-ol (1:1:1 v/v/v)

Evaluation of Data

The measured ion currents I_i of a mixture for the included substances were recalculated on the relative ion current scale – $I_{i,\text{rel}}$ (relative to I_i of the base peak in MIMS spectrum of mixture) and a system of linear equations was obtained (according to Eq. (10)).

For evaluation of relative concentrations of individual compounds in mixtures, Microsoft Excel Solver was used. MS Solver uses a multiparameter adjustment by the nonlinear least-squares method using the Levenberg–Marquardt algorithm. The Solver found the minimum of the sum of the squares of the residuals (\ddot{A})

$$\ddot{A} = a_{ij}^{\text{exp}} - a_{ij}^{\text{calc}} \quad (11)$$

for systematically varied relative concentrations $c_{j,\text{rel}}$. Relative concentrations of individual species in sets I and II obtained by the described procedure are summarized in Table II (aromatics) and Table III (alcohols), respectively.

The measured spectra of set I were compared with those of pure substances at different total experimental molar concentrations (Fig. 6) and the molar concentration ratio of benzene: toluene: *p*-xylene was determined as 0.85:1:0.99 (Table II – overall result). It is important to note that the experimental molar concentration ratio of benzene, toluene and *p*-xylene in solution below the membrane was 1:0.84:0.74, so we can assume that the

TABLE II
Calculated relative concentration of components in set I^a

$c_{\text{m}}, \text{ mmol l}^{-1}$	Benzene	Toluene	<i>p</i> -Xylene
0.58	0.4913	0.4732	0.6152
1.16	0.4616	0.5232	0.5177
1.74	0.4863	0.5125	0.5524
2.89	0.4257	0.5287	0.5123
4.05	0.4026	0.5653	0.4695
5.21	0.4192	0.5677	0.4864
Average	0.4478 ± 0.034	0.5284 ± 0.0322	0.5251 ± 0.0477
After normalization	0.85	1	0.99

^a c_{m} is the sum of molar concentrations of components.

pervaporation of nonpolar compounds in set I through the membrane was not significantly influenced by the presence of the membrane (Fig. 9A). If the deviations of evaluated relative molar concentrations of benzene, toluene and *p*-xylene for different total molar concentration are taken into account (see Table II – partial results), the results are only slightly different.

Based on our results it can be concluded that the multicomponent analysis can be applied to pervaporation of mixtures of nonpolar compounds. This analysis enables the determination of compounds (intermediates, products) according to specific ion currents of given *m/z* present in the solution below the membrane and their relative concentration in solution.

The measured spectra of set II were compared with those of pure substances at different total molar concentrations and the molar concentration ratio of methanol–ethanol–propan-1-ol was determined as 0.087:0.89:1 (Table III – overall result). The experimental, preset ratio of molar concentrations of methanol–ethanol–propan-1-ol was 1:0.69:0.48.

Due to the large dissimilarity of the ratios of calculated and experimental relative concentrations for polar compounds (Fig. 9B), we assume that PTFE membrane, which is permeable especially to nonpolar compounds, could significantly influence the amount of pervaporation of set II through the

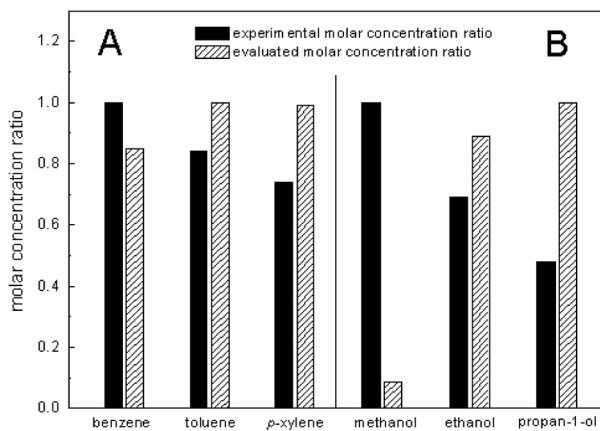


FIG. 9

The comparison of experimental molar concentration ratio of benzene, toluene and *p*-xylene (which was 1:0.84:0.74) to evaluated molar concentration ratio of benzene, toluene and *p*-xylene (0.85:1:0.99) in benzene–toluene–*p*-xylene (A) and the comparison of experimental molar concentration ratio of methanol, ethanol and propan-1-ol (which was 1:0.69:0.48) to evaluated molar concentration ratio of methanol, ethanol and propan-1-ol (0.087:0.89:1) in methanol–ethanol–propan-1-ol (B)

membrane. Moreover, the measured spectra of pure methanol show that only a small portion of methanol pervaporates through the membrane. The methanol concentration detected in MS is 1:0.087 less than the real concentration in solution of set II. Hence, methanol pervaporates poorly through the membrane because of its high polarity. The results show that propan-1-ol penetrates more than ethanol and also more than methanol.

TABLE III
Calculated relative concentration of components in set II^a

c_m , mmol l ⁻¹	Methanol	Ethanol	Propan-1-ol
0.00875	0.0405	0.4193	0.5214
0.01801	0.0427	0.4396	0.5002
0.02646	0.0441	0.4436	0.4943
0.04374	0.0430	0.4422	0.4960
0.0611	0.0442	0.4494	0.4886
0.079	0.0453	0.4564	0.4809
Average	0.0433 ± 0.0015	0.4418 ± 0.0114	0.4969 ± 0.0125
After normalization	0.087	0.89	1

^a c_m is the sum of molar concentrations of components.

We can see that the membrane plays an important role for the amount of pervaporating substances. The reason for discrepancies could be high polarity of alcohols, especially in the case of methanol. Another reason can be the unfulfilled assumption of independent vapor permeation through the membrane of polar substances in a mixture. This suggests the independence of pervaporation of substances on fragmentation of their molecules in ionic source (fragmentation is influenced by the concentration of substances in solution). However, some substances penetrate poorly through the membrane and only a small part of molecules in solution is getting to ionic source and is detected. The amount of ion currents is less than expected. The multicomponent analysis of a mixture of compounds after pervaporation through a PTFE membrane is suitable only for a mixture of nonpolar substances.

This research was supported by the Research Project Inchembiol MSM0021622412 and COST OC 174.

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