SIGNAL TRANSFER BY CHEMICAL SYSTEMS

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Abstract

An attempt is made to apply the cathegories of the information and measurement theories to chemical systems. At first the characterization of the quality of a chemical signal is given. This property is also quantitatively expressible by the here defined "chemical frequency". Further, a short survey deals with the chemical multiplex and MODEM systems. Some examples present the chemical signal processing and data transfer.

Keywords: chemical system simulation, chemical frequency, chemical amplification

List of the applied symbols

A amplification (effective)
B reacting substance
c chemical concentration
f_c chemical frequency
G product substance
I electric current
I_n mol stream
I_v volume stream
j imaginary unit
M_r relative molecular mass
p pressure
r coupling coefficient
U voltage
β stoichiometric coefficient
γ stoichiometric coefficient
ε_r relative dielectric constant
μ amplification

Introduction

Signal processing of our days is dominated by electrical processing over pneumatic and hydraulic ones.

In the measurement theory the signals are generally characterized by the following fundamental properties:

— amplitude
— power
— time dependence
— frequency spectrum.

Amplitudes are either fluxi or potentials. Amplitudes and powers of the physical signals can be expressed as follows:

		electric signal	pneumatic signal
amplitude	(fluxus)	current I [A]	volume stream I_V [$m^3 \cdot s^-$]
	(potential)	voltage U [V]	pressure p [$N \cdot m^{-2}$]
power		$I \cdot U$ [W]	$I_V \cdot p$ [W].

The chemical signal has also a physical quality. The amplitudes are generalized fluxi and potentials [3]. The physical characteristics of chemical signals are:

amplitude	(generalized fluxus)	I_n [$mol \cdot s^{-1}$]
	(generalized potential)	c [$mol \cdot m^{-3}$]
power	(generalized)	$P_n = I_n c$ [$mol^2 \cdot m^{-3} \cdot s^{-1}$].

The chemical quality of a chemical signal

The chemical quality of a chemical species can be characterized by the following properties:

— molecular mass (relative molecular mass, M_r)
— polarity (e.g. relative dielectric constant ε_r for dielectrics, standard electrode potential for ions)
— sterical structure of the molecule.

A signal becomes selective when it is transferred to a chemical compound. This way the compound becomes a *chemical carrier* of the signal (e.g. the reaction product is the carrier of the rate of conversion for tube reactors). The phenomenon is very similar to the carrier frequency applied for electric signals. There, a carrier frequency can be chosen for the signal in the $(0, \infty)$ region to distinguish it from other signals.

For non-ionic chemical species (compounds, radicals) a dimensionless complex quantity can be introduced, the *chemical frequency*.

$$f_C = M_r + j\varepsilon_r \tag{1}$$

characterizing the chemical carrier. In the $\varepsilon_r - M_r$ plane a point corresponds to the compound. The sterical structure gives the possibility of a finer distinction at a certain chemical frequency and is comparable to the phase of the electric signals.

When applying chemical carriers, the common transport of several pieces of information is possible in the same tube in liquid or in gas phase, provided the compounds do not react with one another. This is a complete analogy with the transfer of several electric signals by different carrier frequencies along the same wire with not overlapping frequency bands.

Chemical signal processing

Chemical carriers form typical multiplex systems. All equipments are *multiplexers* separating the chemical compounds according to the real or/and imaginary part of the chemical frequency. This way the signals which have been run side by side separate and turn into a series of signals following one another. Equipments having this property are the various chromatographs, the electrophoretometers, etc. Gel permeation chromatographs separate by the real part (M_r), adsorption chromatographs separate by the imaginary part (ε_r). The mixing of the compounds can be considered as a demultiplexing process.

Molecular sieves and adsorbents are in accordance with our concept *filters*. Sieves are low-cut filters in the real part of f_C (Fig. 1), while selective adsorbents are *nutches* in the imaginary part (Fig. 2). The Figure 1 and 2 show the state functions.

The true chemical signal procession is the chemical reaction. We shall call the spot where the chemical reaction proceeds reactor regardless whether there is a reactor vessel present or not. The reactor plays the same role in the chemical

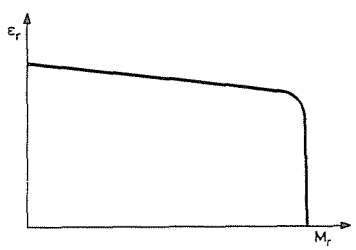


Fig. 1. State function of a molecular sieve

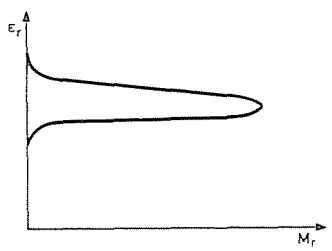


Fig. 2. State function of a selective adsorbent

signal processing as the processor of the computer in the digital electric systems.

In a chemical reactor one or more chemical qualities are generated from one or more other chemical qualities. A chemical reaction can be given by the reaction

$$\sum_{r=1}^{n} \beta_r B_r = \sum_{s=1}^{m} \gamma_s G_s. \tag{2}$$

where β_r stands for the stoichiometric number of the reacting (input) substance, B_r, γ_r labels that of the reaction product (output substance) G_s. *A* very simple example is where both n and m are equal to 1. In this case the indices may be omitted and the equation of the signal transfer has the form

$$\beta c_B^0 = \gamma c_G^0. \tag{3}$$

where c_B^0 is the initial concentration of B, while c_G^0 is the concentration of G for complete transformation. The amplification in this reaction is

$$\mu_{G/B} = \frac{c_G^0}{c_B^0} = \frac{\beta}{\gamma}. \tag{4}$$

This is the possible maximal amplification, the amplification factor. If the reaction proceeds only to a given conversion the amplification can be calculated taking into account the equation

$$\beta c_B^0 = \beta c_B + \gamma c_G. \tag{5}$$

where c_B and c_G are intantial concentrations. Substitution of Eq. (4) into Eq. (5) gives

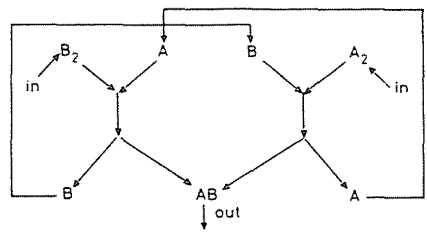
$$c_G = \mu_{G/B}(c_B^0 - c_B). \tag{6}$$

The effective amplification is therefore

$$A_{G/S} \equiv \frac{c_G}{c_B} = \mu_{G/B}\left(1 - \frac{c_B}{c_B^0}\right) \tag{7}$$

In a similar way calculations can be carried out for any types of reactions.

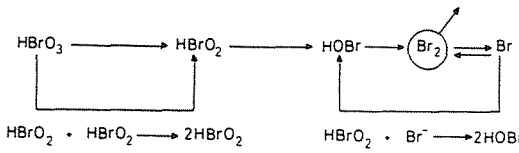
Time-dependent amplification may occur in autocatalytic processes, since feed-back is needed. A very simple feed-back process is the following [2]:



(8)

This is the scheme, for example, for the association of chlorine and hydrogen to hydrogenchloride.

A special case of such reactions is where the amplification is a periodic function of the time since the product concentration changes periodically in time. Lotka-Volterra reactions show such properties. The Zhabotinsky reaction [5] is a real Lotka-Volterra reaction:



(9)

Physical—chemical signal coupling

A signal can be transferred from a physical carrier to a chemical one if the physical signal can produce a chemical reaction. In the opposite direction, a signal can be transferred from a chemical carrier to a physical one, if a chemical reaction or a change in concentration or mass current produce a physical change.

The transfer from physical to chemical carrier can be considered as a modulation of the signal, which after a signal processing can be retransferred, i.e. demodulated. This way we have a complete MODEM system.

The transfers can be of fluxus-fluxus (I/I), fluxus-potential (I/U), potential-fluxus (U/I) potential-potential (U/U) type. For idealized transformers Onsager's reciprocity relations [1, 4] are valid and for linear cases we have for the coupling coefficients

$$\begin{bmatrix} U_{\text{phys}} \\ I_{\text{phys}} \end{bmatrix} = \begin{bmatrix} r & 0 \\ 0 & 1/r \end{bmatrix} \begin{bmatrix} c \\ I_n \end{bmatrix}. \tag{10}$$

When a physical signal acts locally, the chemical answer is the integration of the signal: the local concentration increases. Otherwise, in a flowing system the chemical signal appears as a mass stream.

Now some examples for the physical to chemical coupling are presented.

Electric current gives rise to anodic oxidation and cathodic reduction. The rate of the concentration change is proportional to the current intensity.

Light (mainly ultraviolet light) initiates chemical reactions (e.g. chlorination of aromatics). The rate of concentration change in static system or the intensity of mass current in streaming system is proportional to the light intensity.

In the receptors of the eyes the light current produces a chemical change (rodopsine to opsine [1]). According to the experiments the stimulus caused by the light is a logarithmic function of the light intensity.

Living creatures transform mechanical pressure and pressure differences into stimuli. The answers of the organism are ache sensation and sound sensation, respectively. These stimuli propagate in the organism as chemical signals (mass transport) or integrate locally (increase of concentration).

There are also examples for the chemical to physical coupling. Some chemical reactions produce light. There are reactions with gaseous products, therefore the output signal is either pressure (potential type amplitude) or volume stream (fluxus). There are a lot of internal or external motions in organisms, e.g. the increasing of the cross-section of the blood-vessels by increasing the coffein concentration.

Parallel signal transfer

The transfer of several chemical signals on the same physical channel ("tube") is important above all in superior living creatures. Physical channels can be blood- and lymphatic vessels, veins in plants, etc. In these vessel systems endochrinic glands send control signals and information to different parts of the organism and receive answer signals from them. The signal is represented by a mass stream (or local concentration) and the steric structure of the molecule (hormons, coenzymes, etc.). In the vessel liquor several signal carriers move parallelly. The information is received by selective detectors on the cell wall (the selectivity is not perfect, this is the reason of the poisonibility with compounds of similar structure). The detectors are sensitive to the polarity and the steric structure of the molecule. The intensity of the detected signal changes monotonously with the local concentration of the carrier compound in the vein solution. Because of the finite number of detectors a saturation effect is observable.

The signal transfer from the cell wall to the cytoplasme can take place with several mechanisms. An interesting possibility of the molecule transport through the membrane is the so-called pendulum mechanism [1]. Fig. 3 shows

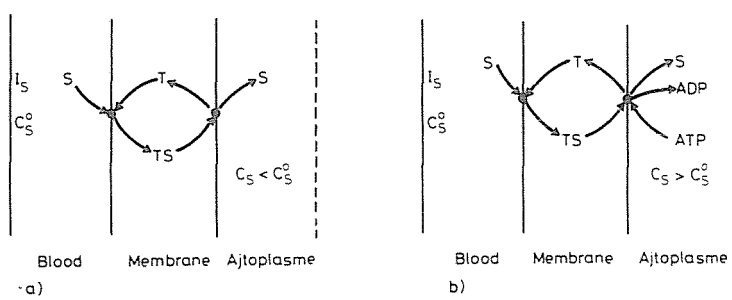


Fig. 3. Mass transports through the cell wall; a: passive, b: active transport

the possible variants of the mass transport. When the concentration c_S of the carrier substance in the cytoplasme is lower than that in the vein (c_S^0) the transport is passive, the substance S attaches selectivity to the transport protein T and the complex dissociates on the other side of the cell wall, at the cytoplasme. In the opposite case ($c_S > c_S^0$) additive energy is necessary to the mass transport which is supplied by an adenozine-triphosphate (ATP) molecule. This is an active mass transport.

Multicomponent gases, liquids and solutions often have to be separated. The purpose can be the separation itself (e.g. hypersorber) or the analysis of the mixture (gel permeation, adsorption and ion exchange chromatographies, electrophoresis). It is satisfactory sometimes to separate only by the molecular mass or by the polarity. In many cases, however, if a series of similar compounds is present in the mixture (e.g. degradation products of fats) a common application of both methods (after one another) is advisable. In this case the resolution on the state surface increases considerably. In the region of operation $\Delta f_C = \Delta M_r + j \cdot \Delta \varepsilon_r$ the resolution increases from $\delta M_r + j \cdot \Delta \varepsilon_r$ or from $\Delta M_r + j \cdot \delta \varepsilon_r$ to $\delta f_C = \delta M_r + j \cdot \delta \varepsilon_r$ (Fig. 4).

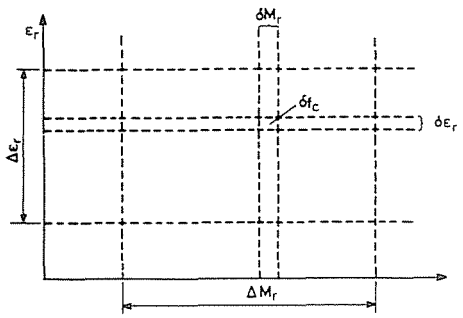


Fig. 4. The common application of gel permeation and adsorption chromatographies

Conclusions

According to the developed theory the chemical signal processing forms a complete multiplex system. When a chemical carrier is applied for distinguishing physical signals the system is similar to the electric signal modulation (carrier frequency) and we have a MODEM system. Graphs of such a system can also be constructed (Fig. 5).

It has been shown that the information and the measurement theories can be adopted to the signal carrying chemical systems, i.e. these systems can be considered like other signal processing systems. Since this kind of systems can be found mostly in living organisms we think the theory can find applications primarily in the study of biological systems.

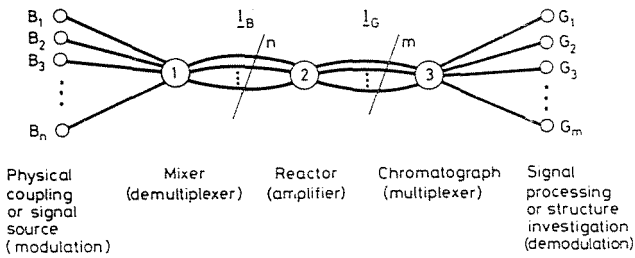


Fig. 5. The graph of a complete chemical multiplex system

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