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MATHEMATICAL CORRELATION BETWEEN MASS TRANSFER COEFFICIENTS AND PARAMETERS INFLUENCING THE PENICILLIN G REACTIVE EXTRACTION PROCESS

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ABSTRACT. In this paper a correlation between the individual mass transfer coefficient of Penicillin G for the aqueous phase and two parameters of the reactive extraction process of Penicillin G with Amberlite LA-2, namely the extractant concentration in the organic phase, and the mixing intensity, was established. The proposed correlation offers a good concordance with the experimental values of the mass transfer coefficient and may be applied with a maximum error of 18 % and an average deviation of 1.6 %.

RESUMO

O presente trabalho estudou vários procedimentos para a extração da Penicilina G . Foram determinados parâmetros para o processo de extração reativa da Penicilina G com Amberlite LA- 2, especificamente a concentração de extratante na fase orgânica e a intensidade de mistura. A correlação entre o coeficiente de transferência de massa da Penicilina G da fase aquosa e os dois parâmetros em acetato de butila também foi determinado. Esta correlação foi boa e pode ser aplicada com um erro experimental, máximo de 18% e um desvio padrão de 1,6%..

KEYWORDS : Penicillin G extraction, reactive extraction, Amberlite LA-2, mass transfer coefficients.

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INTRODUCTION

The Penicillin G obtained by biosynthesis is separated from the aqueous phase by means of some laborious extraction and reextraction stages, resulting finally in an overall separation yield of 70 - 75 %.[1] In order to eliminate these shortcomings the authors have studied the possibility of the Penicillin G separation by means of other procedures, the reactive extraction among them. The conditions of the reactive extraction process have previously been established.[2, 3] These studies have demonstrated the significant influence of the extracting agent concentration in organic phase and of the mixing intensity.

This paper is aimed to settle a correlation between the Penicillin G individual mass transfer coefficients and the variables influencing decisively the reactive extraction process (the extractant concentration value in solvent, the mixing intensity value) using an extractant of the Amberlite LA-2 type in butyl acetate medium.

EXPERIMENTAL

The laboratory equipment used (figure 1) consists of a glass column of 56 mm inner diameter and 180 mm height, provided with a jacket through which the thermosetting agent passes, namely water maintained at 25 °C by means of a thermostat. The two phases were mixed together by a vibratory mixer with a perforated disk of 45 mm diameter having a 17 % free section. The vibrations had a frequency of 50 Hz and a variable amplitude.

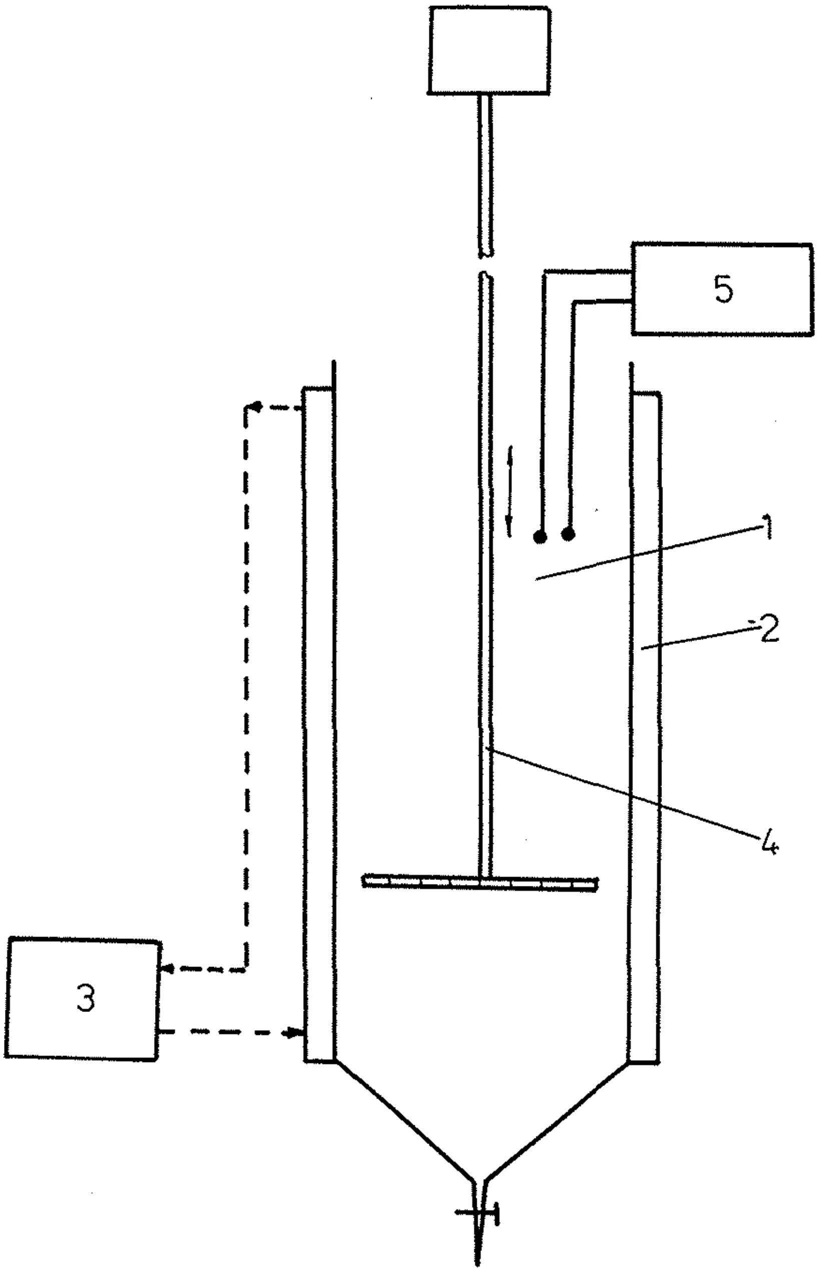

Figure 1. The experimental equipment. 1 - glass column; 2 - jacket; 3 - thermostat; 4 - vibratory mixer; 5 - pH-meter.

The resulting emulsion was separated in a centrifugal separator.

The experimental studies on Penicillin G reactive extraction were carried out in a batch system. In this work Penicillin G potassium salt was used. Its initial concentration in aqueous phase was of 7.7 g L^{-1}. The Amberlite LA-2 concentration values in butyl acetate phase was 64, 92 and 166 g L^{-1}. The volume ratio of organic phase and aqueous phase was 1 : 2, namely 50 mL solvent and 100 mL Penicillin G potassium salt aqueous solution.

The pH adjustement of the initial aqueous solution, at pH = 3, was made by means of 5 % sulphuric acid solution added in function of the prescribed pH - value measured by a digital pH - meter.

The intensity values of the two phases mixing, calculated by the relationship :

$$i = A \cdot f$$

was varied between 0.025 and 0.25 m s^{-1}.

The process development was followed by dosing the Penicillin G by the iodometric method.

RESULTS AND DISCUSSION

The separation process by reactive extraction can be controlled by diffusion or by the chemical reaction. The extraction rate determining step can be established by means of the influence of the mixing intensity on the reactive extraction yields, for a certain extracting agent concentration. The increase in the Penicillin G extraction yield with the increase in the mixing intensity value shows that the Penicillin G diffusion is separation rate determining step. For higher mixing intensity values the reactive extraction yield become almost constant, in this case the chemical reaction being the determining step. The results obtained for three Amberlite LA-2 concentrations are plotted in Figure 2.

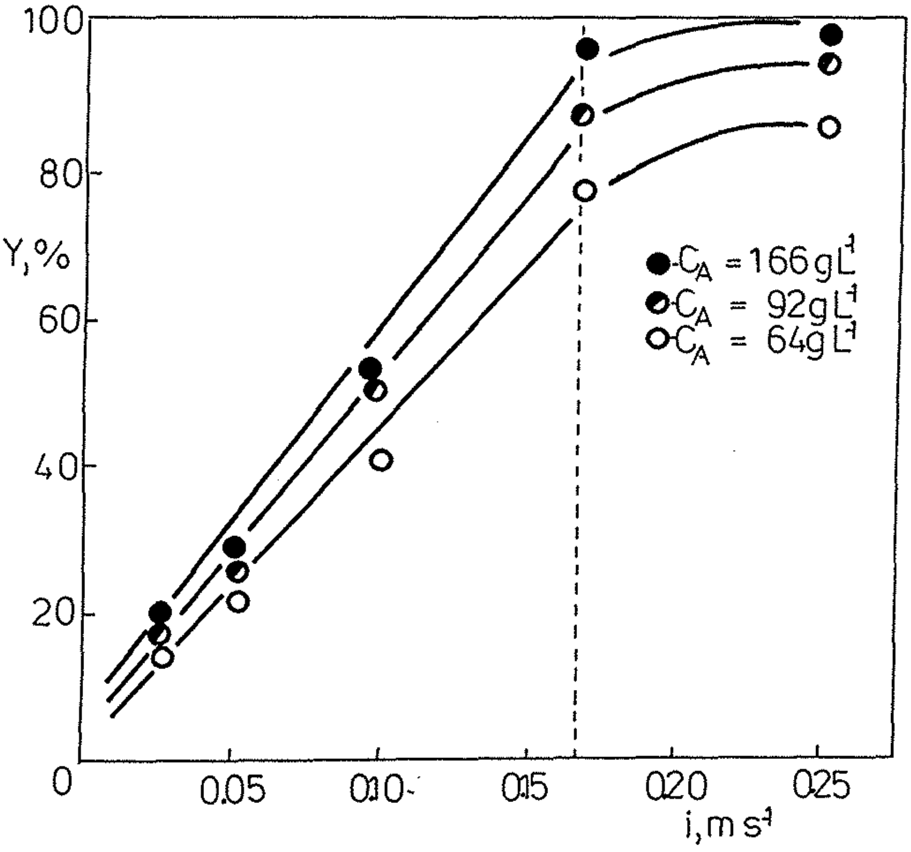

Figure 2. The reactive extraction yield versus mixing intensity.

As seen in Figure 2 the yield increases rapidly within the mixing intensity range 0.025 - 0.165 m s^{-1}, for any extracting agent concentration. For this intensity range the Penicillin G mass transfer is reactive extraction rate determining step. Over 0.165 m s^{-1} value the chemical reaction controls the separation process.

The correlation between Penicillin G individual mass transfer coefficients for the aqueous phase and Amberlite LA-2 concentration and mixing intensity was settled for the mixing intensity values bellow 0.165 m s^{-1}. The mass transfer coefficient values were calculated by the method proposed in previous papers.[2] Thus, by plotting ln Cp in function of extraction time for several mixing intensity values the straight lines have been obtained. The values of the individual mass transfer coefficients were estimated by means of straight line slopes. For this purpose, the reactive extraction yields were calculated for several extraction time values, at three extracting agent concentrations and four mixing intensity values. The obtained values are given in Table 1.

Taking in account the tabulated data, the values of the Penicillin G individual mass transfer coefficients for the aqueous phase were estimated by means of straight line slopes plotted in Figures 3, 4 and 5.

The values of these coefficients are given in Table 2.

As it was to be expected, the Penicillin G individual mass transfer coefficient increases rapidly with the increase of the considered parameters values. With an increase of 2.6 times of Amberlite LA-2 concentration in butyl acetate combined with an increase of 6.6 times of mixing intensity the mass transfer coefficient value are seen to increase about 15 times.

The following relationship was proposed between the individual mass transfer coefficient and the two process variables :

$$k_p = a \cdot C_a^b \cdot i^c$$

Table 1. The reactive extraction yield values in function of extraction time, at several extracting agent concentrations and several mixing intensity values..

C_A, $g\,L^{-1}$	i, $m\,s^{-1}$	extraction time, s						
		5	10	15	30	45	60	90
64	0.025	13.9	13.9	14.0	14.3	15.0	16.3	18.1
	0.050	16.8	18.1	19.2	19.5	20.0	21.0	24.2
	0.100	32.4	33.6	34.5	35.3	37.3	39.3	40.8
	0.165	75.0	76.3	77.0	78.8	79.8	82.5	90.0
92	0.025	14.4	15.2	15.8	16.8	17.3	18.5	19.1
	0.050	19.0	20.5	21.2	22.3	23.0	24.5	26.0
	0.100	37.1	39.8	40.2	41.3	42.5	46.1	47.8
	0.165	78.5	82.7	84.3	86.0	88.2	90.0	91.3
166	0.025	16.4	18.3	18.9	19.1	19.5	20.4	21.1
	0.050	21.3	22.8	23.2	24.1	25.0	26.8	27.2
	0.100	42.9	43.2	43.7	44.3	45.3	51.7	53.0
	0.165	87.1	89.0	89.4	90.1	91.9	93.5	94.9

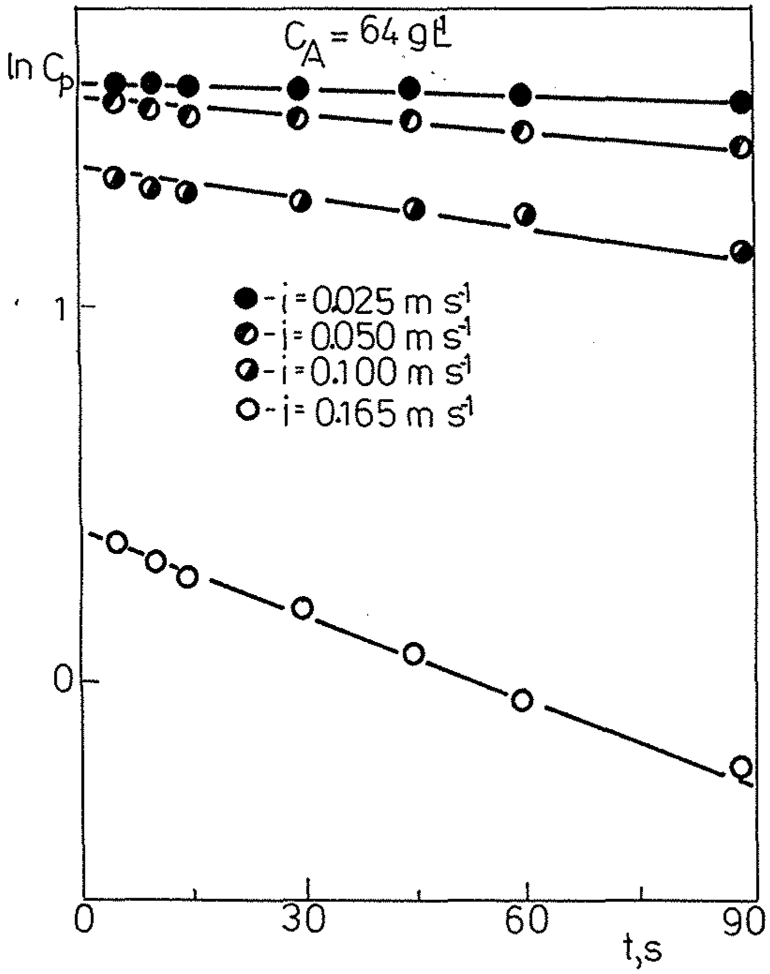

Figure 3. ln C_p versus mixing time for C_A = 64 g L^{-1}.

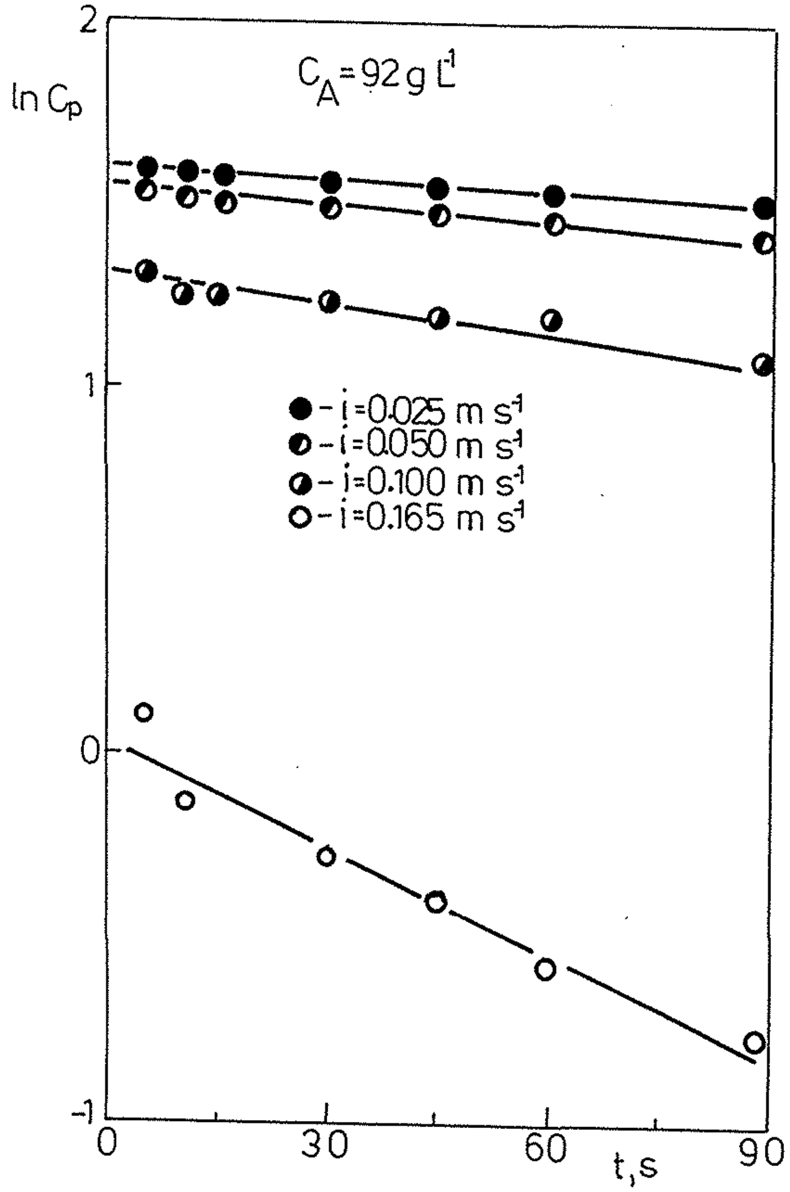

Figure 4. ln C_p versus mixing time for $C_A = 92\ g\ L^{-1}$.

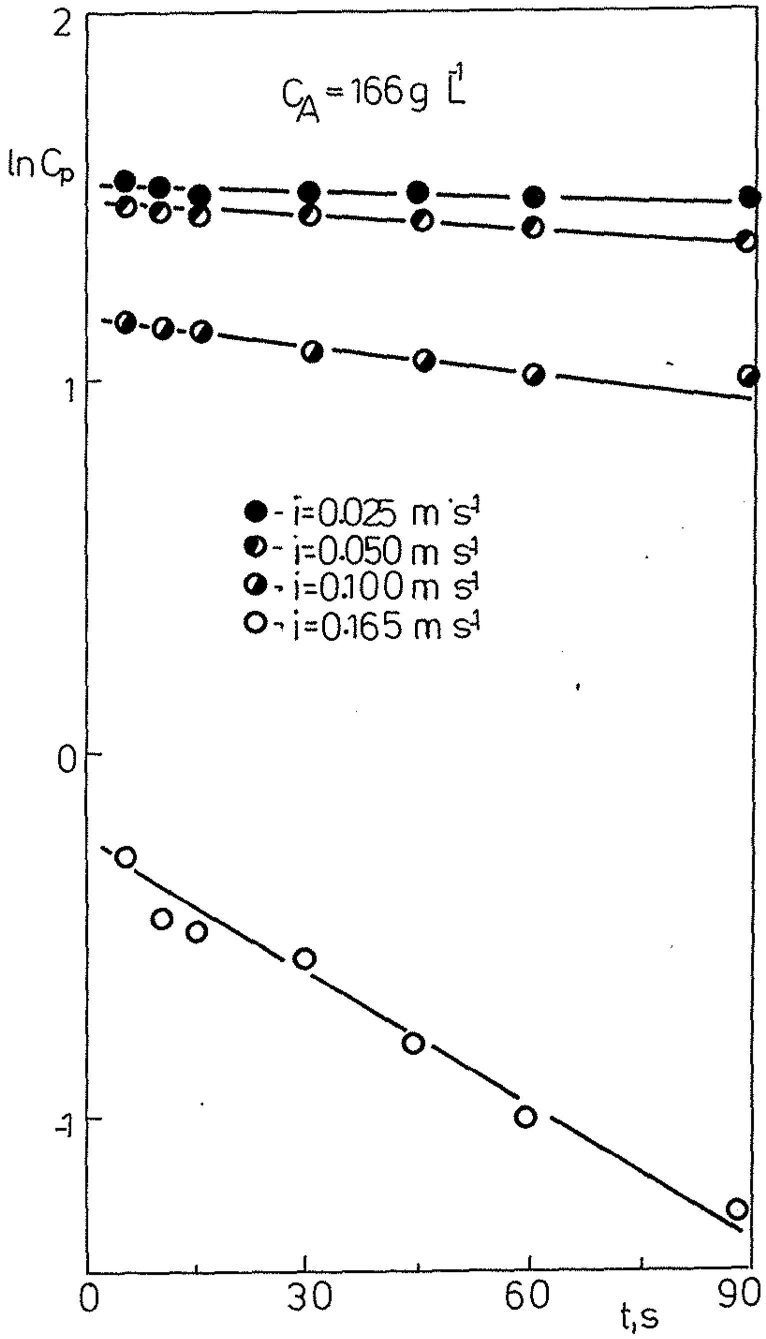

Figure 5. ln C_p versus mixing time for C_A = 166 g L^{-1}.

Table 2. The Penicillin G individual mass transfer coefficient values for the aqueous phase.

C_A,	$k_P \times 10^3$, s^{-1}			
$g\,L^{-1}$	$i = 0.025\ m\,s^{-1}$	$i = 0.050\ m\,s^{-1}$	$i = 0.100\ m\,s^{-1}$	$i = 0.165\ m\,s^{-1}$
64	1.00	1.75	3.90	7.00
92	1.15	2.60	6.40	11.25
166	1.30	3.10	7.70	14.80

The coefficient a and the exponents b and c were determined by linearizing,[4] for constant values of the extractant concentration, using the following relation :

$$k_p = a' \cdot i^c$$

$$\text{or} \quad \ln k_p = \ln a' + c \cdot \ln i$$

where $a' = a \cdot C_A^{\ b}$. By plotting ln k_p in function of ln i for the three concentration values of the extractant have been obtained the straight lines illustrated in Figure 6.

Thus, the following expressions can be written by means of these straight lines :

$$k_p = 0.046 \cdot i^{1.08} \qquad \text{for } C_A = 64\ g\,L^{-1}$$

$$k_p = 0.095 \cdot i^{1.20} \qquad \text{for } C_A = 92 \text{ g L}^{-1}$$

$$k_p = 0.150 \cdot i^{1.30} \qquad \text{for } C_A = 166 \text{ g L}^{-1} .$$

As can be observed, both the coefficient a' and the exponent c are influencing by the Amberlite LA-2 concentration. In order to settle this influence it was plotted a' and c values in function of extracting agent concentration obtaining two straight lines given in Figure 7.

These straight lines equations are :

$$a' = 0.91\text{x}10^{-3}\, C_A$$

$$c = 1 + 1.77\text{x}10^{-3}\, C_A$$

Now, the following correlation existing between the Penicillin G individual mass transfer coefficients for the aqueous phase and the Amberlite LA-2 concentration in butyl acetate and the mixing intensity can be written :

$$k_p = 0.91\text{x}10^{-3}\, C_A \cdot i^{1 + 1.77\text{x}10^{-3}\, C_A}$$

By using this relationship the theoretical values of Penicillin G individual mass transfer coefficients have been calculated. In Table 3 are presented the theoretical values and the ratio of theoretical and experimental values .

The proposed correlation offers a good concordance with the experimental values of mass transfer coefficients with an average deviation of 1.6 % and a maximum error of 18 %, as can be seen in Table 3.

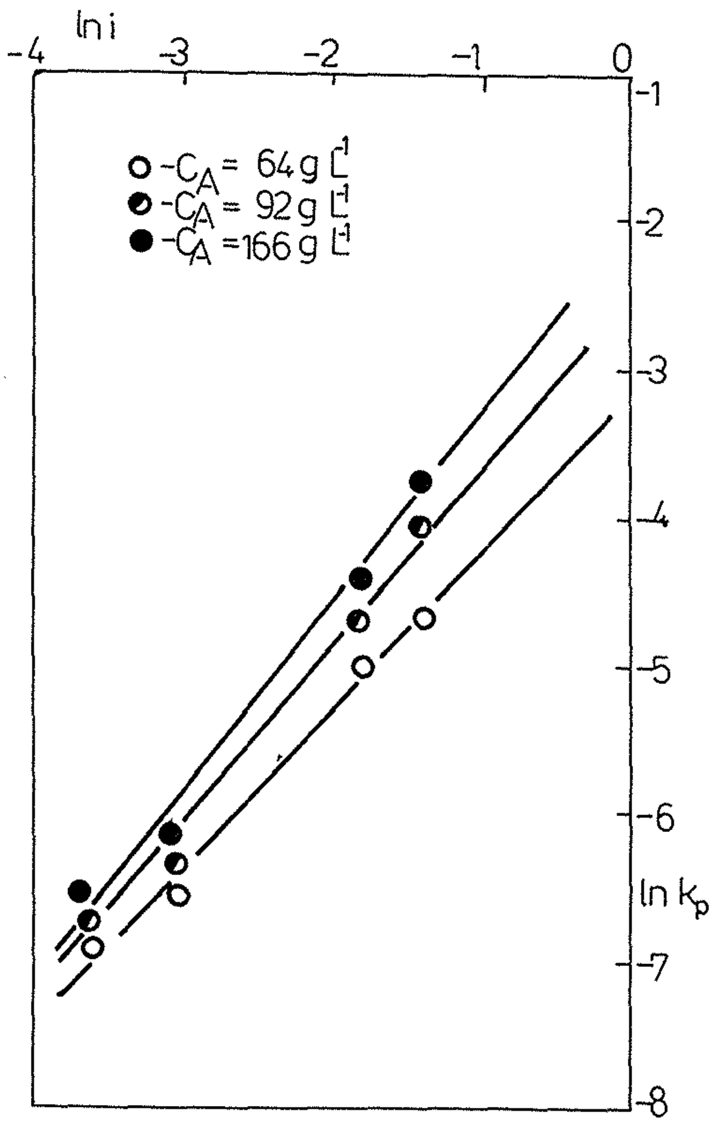

Figure 6. ln i versus ln k_p.

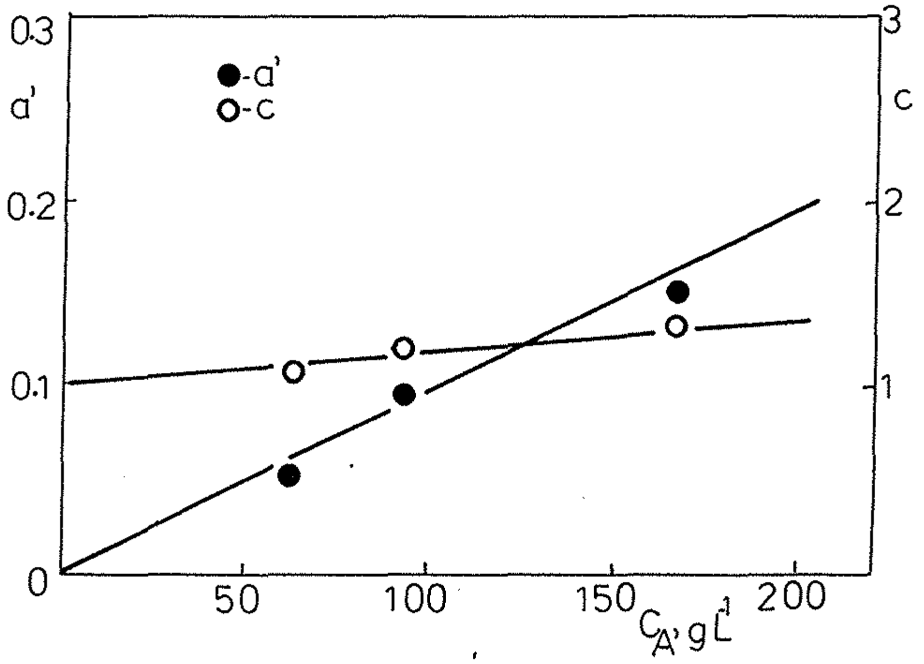

Figure 7. The influence of extracting agent concentration on coefficient a' and exponent c.

Table 3. The experimental and the theoretic values of the Penicillin G individual mass transfer coefficient for the aqueous phase.

C_A, g L^{-1}	i, m s^{-1}	k_P x10^3, s^{-1}	k_{Pt} x10^3, s^{-1}	k_{Pt} / k_P	r_{med}
64	0.025	1.00	0.96	0.96	1.016
	0.050	1.75	2.07	1.18	
	0.100	3.90	4.48	1.15	
	0.165	7.00	7.83	1.11	
92	0.025	1.15	1.15	1.00	
	0.050	2.60	2.57	0.99	
	0.100	6.40	5.75	0.90	
	0.165	11.25	10.30	0.92	
166	0.025	1.30	1.28	0.98	
	0.050	3.10	3.13	1.01	
	0.100	7.70	7.68	0.997	
	0.165	14.80	14.68	0.999	

CONCLUSIONS

For the mixing intensity values range bellow 0.165 m s^{-1} the Penicillin G diffusion is the reactive extraction process rate determining step. Over this value, the chemical reaction controls the separation process.

The proposed correlation between the Penicillin G individual mass transfer coefficients for the aqueous phase and the Amberlite LA-2 concentrations in organic phase and the mixing intensity values offers a quantitative description of the influence of these two parameters on reactive extraction process.

The aim of the future studies is to develop this correlation with the terms describing the pH - value, the volume ratio and the Penicillin G initial concentration influences.

List of Symbols

C_p - Penicillin G concentration, g L^{-1};

C_A - extracting agent concentration, g L^{-1};

k_p - Penicillin G experimental individual mass transfer coefficient for the aqueous phase, s^{-1};

k_{pt} - Penicillin G theoretical individual mass transfer coefficient for the aqueous phase, s^{-1};

i - mixing intensity, m s^{-1};

A - vibration amplitude, m;

f - vibration frequency, Hz;

r - ratio of theoretical and experimental mass transfer coefficients values;

t - extraction time;

Y - reactive extraction yield, %.

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