ХИМИЯЛЫҚ ТЕХНОЛОГИЯ ЖӘНЕ ЭКОЛОГИЯ
ХИМИЧЕСКАЯ ТЕХНОЛОГИЯ И ЭКОЛОГИЯ

Study of calculation of operating extracting problems with multi-stage countercrent in part-dissolved system based on Excel

Excel негізінде жартылай еріген жүйедегі көпсатылы қарсыағынды экстракцияны есептеу жұмыстарын зерттеу

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Мақалада Excel бағдарламасының көмегімен 50 %-ды ацетон–хлороформ ерітіндісінен ацетонның қарсыағынды экстракция процесінің негізгі көрсеткіштері есептелген. Сұйықтық экстракция фармацевтикалық өндірісте, химиялық технологияда және металлургияда сұйық қоспаларды бөлу үшін кең қолданылады. Сулы экстракт ацетон–хлороформ жүйесі үшін қарсыағынды экстракция процесінің регрессия теңдеуі алынған. McCabe-Thiele (сатылап тұрғызу) әдісімен салыстырғанда бұл тәсіл нақтырақ, зерттеу үшін қарапайым және қолдануға қолайлы.

В статье с использованием программы Excel были рассчитаны основные параметры процесса противоточной жидкостной экстракции ацетона из раствора 50 %-го ацетона и хлороформа. Жидкостная экстракция широко применяется в фармацевтической промышленности, химической технологии и в металлургии для разделения жидких смесей. Получено уравнение регрессии для системы водного экстракта ацетон–хлороформ при противоточной экстракции. По сравнению с методом McCabe-Thiele (пошаговое построение) данный метод более точный, прост для изучения и удобен для применения.

0 Preface

The unit operation of liquid-liquid extraction has been used widely in separating liquid mixtures in the pharmaceutical, chemical engineering, metallurgical industries, and so on. As the calculation of the operating type is long to a process of trail and error non-linearly, a simplified graphical procedure for calculating process is adapted for the McCabe-Thiele step-by-step construction. Obviously, this process is tedious, lengthy, time-consuming and inaccuracy. Now, with the help of Microsoft Excel carried more than 200 functions and convenient menus and toolbars instead of program, it can solve the complex engineering problem containing many variables and non-linear [1, 2] using analytical methods. As an example of acetone in the solution of acetone 50 % (w) and chloroform with three theoretical stages countercurrent, in which know the ratio of S/F and X_{Fa} in the feed, it study how to solve this problem analysis with excel the resolving method instead of the plotting method to carry out calculating process automatically.

Overall material balance:

$$F + S = R_3 + E_1 \tag{1}$$

Component A:

$$FX_{Fa} + SZ_a = R_3X_{3a} + E_1Y_{1a} \tag{2}$$

Component S:

$$FX_{Fs} + SZ_s = R_3X_{3s} + E_1Y_{1s} \quad (2)$$

To make material balances for every stage:

$$R_{i-1} + E_i = R_i + E_{i-1} \tag{4}$$

$$R_{i-1}X_{i-1,a} + E_iY_{ia} = R_iX_{i,a} + E_{i-1}Y_{i-1,a} \tag{5}$$

$$R_{i-1}X_{i-1,s} + E_iY_{is} = R_iX_{i,s} + E_{i-1}Y_{i-1,s} \tag{6}$$

Regressing solubility formulas:

$$Y_s = f(Y_a) \tag{7}$$

$$Xs = f(X_a) \tag{8}$$

Distribution formula:

$$Ya = f(Y_a) \tag{9}$$

Normalised formulas:

$$Y_a + Y_b + Y_s = 1 \tag{10}$$

$$X_a + X_b + X_s = 1 \tag{11}$$

$$Z_a + Z_b + Z_s = 1 \tag{12}$$

Stage efficiency η:

$$\eta = R_3X_{3a} / FX_{Fa} \tag{13}$$

1 Mathematical model

Fig. 1 shows the extraction process with three stages countercurrent. Mathematical models needed for calculation are the equation of $FX_{fa}X_{fs}$. Stage efficiency on the third stage is calculated by equation 1.

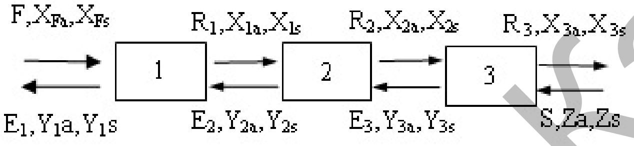


Fig. 1. Schematic of extraction with three stages count-current

2 McCabe-Thiele step-by-step construction

Fig. 2 shows the process of the McCabe-Thiele step-by-step construction for the operating extracting problem. As shown in fig.2, in a triangle phase diagram, first of all, draw solving curves and equilibrium tie lines according to the equilibrium data for the system; secondly, to determine point M according to lever-arm rule and known X_{Fa} and S/F; thirdly, obtain point R_3 on the left of the dissolving curve after assumed $X_{3a}^{\#}$, and point E_3 according to point R_3 through equilibrium tie line; Fourthly, ties points of R_3 and M, and extend its tie line, which intersect point E_1 on the right of solubility curve, determine R_1 according to point E_1

through equilibrium tie line; Fifthly, tie FE_1 and R_3S, after extend them until they intersect point H outside figure on right side; Sixthly, join two points of H and R_1, which intersect with solubility curve and obtain E_2; determine R_2 according to E_2 through equilibrium tie line again; tie H and R_2 which intersect with solubility curve and obtain point E_2.Seventhly, determine R_3 according to E_3 through equilibrium tie line, read the value of X_{3a} according to the new point R_3, after comparing with the value of $X_{3a}^{\#}$. If X_{3a} isn't equal to $X_{3a}^{\#}$, repeat above the process of № 1~7 from the new value of R_3 until X_{3a} is equal to $X_{3a}^{\#}$ or nearly. Finally, find out $X_{3a} = 0.15$, and the third stage efficiency of η is 22.3 %。

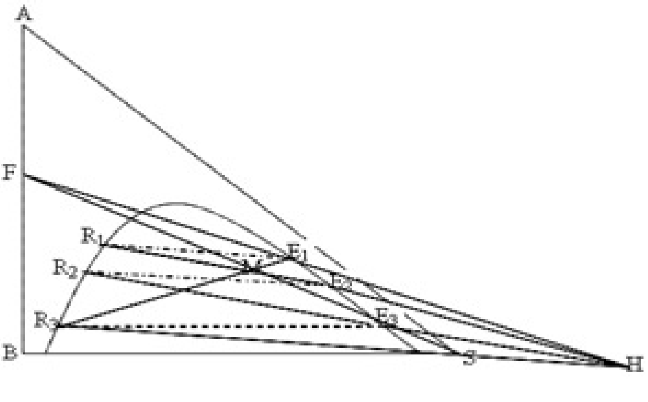


Fig. 2. Constructive step by step of extraction with three-stage countercurrent

3 Analysis method with trail and error based on Excel

3.1 Calculate X_{3a} in the raffinate phase and stage efficiency η as known $F/S=2.1$ and $X_{Fa}=0.5$

Fig.3 shows the calculating process. First of all, regress the phase equilibrium equations of (7) 1 and 2 and distribution equation of 4 according to equilibrium data which are already known [3, 5].

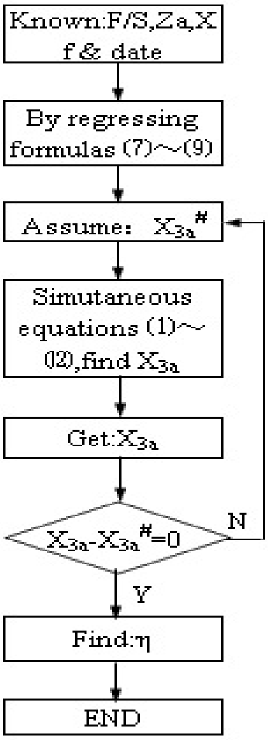
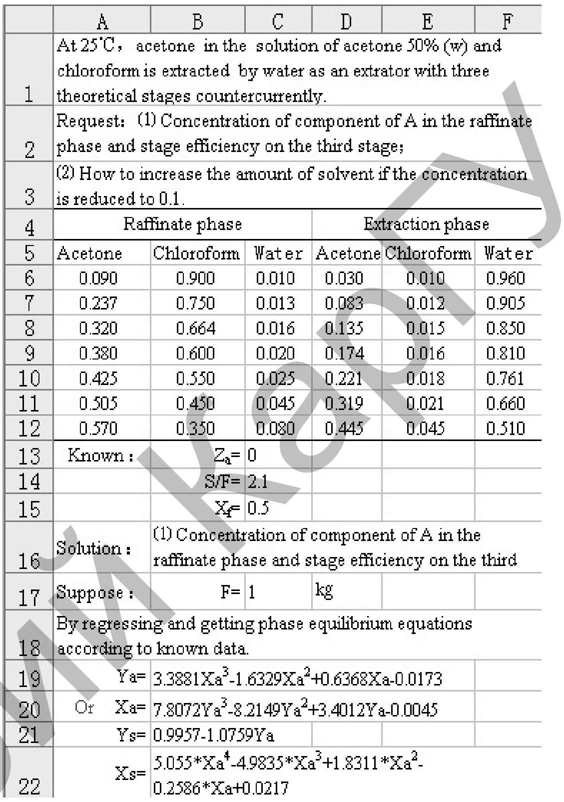
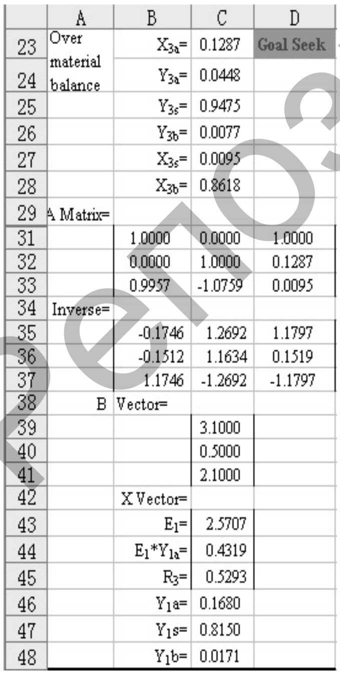


Fig. 3. Schematic of calculation

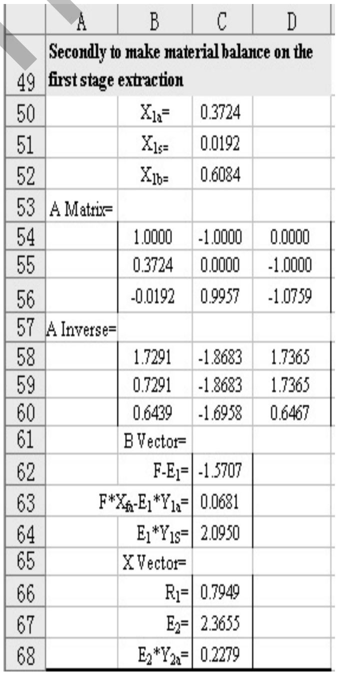


	A	B	C	D	E	F
1	At 25°C, acetone in the solution of acetone 50% (w) and chloroform is extracted by water as an extrator with three theoretical stages countercurrently.					
2	Request: (1) Concentration of component of A in the raffinate phase and stage efficiency on the third stage;					
3	(2) How to increase the amount of solvent if the concentration is reduced to 0.1.					
4	Raffinate phase			Extraction phase		
5	Acetone	Chloroform	Water	Acetone	Chloroform	Water
6	0.090	0.900	0.010	0.030	0.010	0.960
7	0.237	0.750	0.013	0.083	0.012	0.905
8	0.320	0.664	0.016	0.135	0.015	0.850
9	0.380	0.600	0.020	0.174	0.016	0.810
10	0.425	0.550	0.025	0.221	0.018	0.761
11	0.505	0.450	0.045	0.319	0.021	0.660
12	0.570	0.350	0.080	0.445	0.045	0.510
13	Known :	Z_a=	0			
14		S/F=	2.1			
15		X_f=	0.5			
16	Solution :	(1) Concentration of component of A in the raffinate phase and stage efficiency on the third				
17	Suppose :	F=	1	kg		
18	By regressing and getting phase equilibrium equations according to known data.					
19	Ya=	$3.3881Xa^3-1.6329Xa^2+0.6368Xa-0.0173$				
20	Or Xa=	$7.8072Ya^3-8.2149Ya^2+3.4012Ya-0.0045$				
21	Ys=	$0.9957-1.0759Ya$				
22	Xs=	$5.055*Xa^4-4.9835*Xa^3+1.8311*Xa^2-0.2586*Xa+0.0217$				

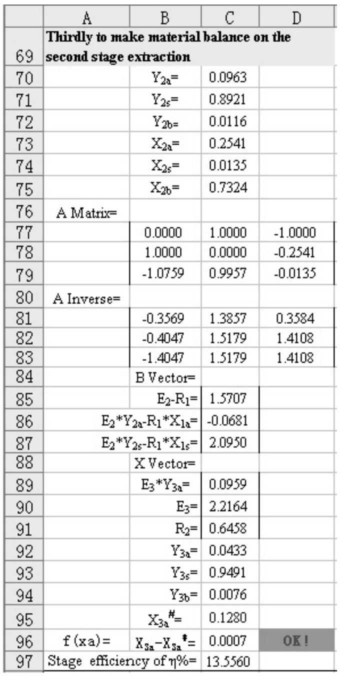
Fig. 4. Question 1 (a)



	A	B	C	D
23	Over material balance	X_{3a}=	0.1287	Goal Seek
24		Y_{3a}=	0.0448	
25		Y_{3s}=	0.9475	
26		Y_{3b}=	0.0077	
27		X_{3s}=	0.0095	
28		X_{3b}=	0.8618	
29	A Matrix=			
31		1.0000	0.0000	1.0000
32		0.0000	1.0000	0.1287
33		0.9957	-1.0759	0.0095
34	Inverse=			
35		-0.1746	1.2692	1.1797
36		-0.1512	1.1634	0.1519
37		1.1746	-1.2692	-1.1797
38	B	Vector=		
39			3.1000	
40			0.5000	
41			2.1000	
42		X Vector=		
43		E_1=	2.5707	
44		E_1*Y_{1a}=	0.4319	
45		R_3=	0.5293	
46		Y_1a=	0.1680	
47		Y_1s=	0.8150	
48		Y_1b=	0.0171	



	A	B	C	D
49	**Secondly to make material balance on the first stage extraction**			
50		X_{1a}=	0.3724	
51		X_{1s}=	0.0192	
52		X_{1b}=	0.6084	
53	A Matrix=			
54		1.0000	-1.0000	0.0000
55		0.3724	0.0000	-1.0000
56		-0.0192	0.9957	-1.0759
57	A Inverse=			
58		1.7291	-1.8683	1.7365
59		0.7291	-1.8683	1.7365
60		0.6439	-1.6958	0.6467
61		B Vector=		
62		$F-E_1$=	-1.5707	
63		$F*X_{fa}-E_1*Y_{1a}$=	0.0681	
64		E_1*Y_{1S}=	2.0950	
65		X Vector=		
66		R_1=	0.7949	
67		E_2=	2.3655	
68		E_2*Y_{2a}=	0.2279	



	A	B	C	D
69	**Thirdly to make material balance on the second stage extraction**			
70		Y_{2a}=	0.0963	
71		Y_{2s}=	0.8921	
72		Y_{2b}=	0.0116	
73		X_{2a}=	0.2541	
74		X_{2s}=	0.0135	
75		X_{2b}=	0.7324	
76	A Matrix=			
77		0.0000	1.0000	-1.0000
78		1.0000	0.0000	-0.2541
79		-1.0759	0.9957	-0.0135
80	A Inverse=			
81		-0.3569	1.3857	0.3584
82		-0.4047	1.5179	1.4108
83		-1.4047	1.5179	1.4108
84		B Vector=		
85		E_2-R_1=	1.5707	
86		$E_2*Y_{2a}-R_1*X_{1a}$=	-0.0681	
87		$E_2*Y_{2s}-R_1*X_{1s}$=	2.0950	
88		X Vector=		
89		E_3*Y_{3a}=	0.0959	
90		E_3=	2.2164	
91		R_2=	0.6458	
92		Y_{3a}=	0.0433	
93		Y_{3s}=	0.9491	
94		Y_{3b}=	0.0076	
95		$X_{3a}^{\#}$=	0.1280	
96	f (xa)=	$X_{3a}-X_{3a}^{\#}$=	0.0007	OK !
97	Stage efficiency of η%=		13.5560	

Secondly find out X_{3a} through solving equations from Eq.1 to Eq.2 simultaneously based on assuming X_{3a}.

For example of the third stage, X_{3a}*is assumed, substituted into Eqs. (3) and (4), and X_{3S} and Y_{3a}.are solved. At the same time, Y_{3s}, Y_{3b} and X_{3b} can be calculated through Eqs.4 of 5 and 6.

Make overall material balance, and find out E_1, R_3 and Y_{1a}.through solving from Eq.7 to Eq.8 simultaneously by the method of inverse matrix.

$$\begin{aligned} F+S &= E_1 + 0 + R_3 \\ FX_{Fa} &= 0 + E_1Y_{1a} + R_3X_{3a} \\ SZ_s &= 0.9957E_1 - 1.0759E_1Y_{1s} + R_3X_{3s} \end{aligned}$$

Acording to matrix of B=AX, there is $X=A^{-1}B$.

$$\text{Then: } B=\begin{vmatrix} F+S \\ FX_{Fa} \\ SZ_s \end{vmatrix},\ A=\begin{vmatrix} 1 & 0 & 1 \\ 0 & 1 & X_{3a} \\ 0.9957 & -1.0759 & X_{3s} \end{vmatrix},\ X=\begin{vmatrix} E_1 \\ E_1Y_{1a} \\ R_3 \end{vmatrix}$$

Similarly, calculate the other parameters of stage 1, 2 and 3 one by one.

Thirdly, compare X_{3a} with X_{3a}^*. As if $X_{3a}-X_{3a}^*$ is 0, this assumption is correct, the stage efficiency η is calculated unless to operate tool of «seek goal» in Excel till $X_{3a}-X_{3a}^*=0$, and get X_{3a}. Fig. 4 shows this process and results in detail. As shown in Fig. 4, to get phase equilibrium equations and distribution equations ($R^2 \geq 0.99$, respectively) putting in rows of 19 to 22 by regressing equilibrium data in list of A5～F12. For example, get $X_{3a}=0.0328$ after to assume $X_{3a}^*=0.18$, and find out Y_{3a}, Y_{3s}, Y_{3b}, X_{3s} and X_{3b} in turn through solving three corresponding inverse matrixes. In D96 input «=IF (ABS (C96) <= 0.0015, «OK!», «FALSE!»)». Here require the goal value in C96 maybe 0.0015. As a result of it shows «FALSE». Operating «goal seek» tool in Excel, C23 is the variable cell, input 0 as a target value in target cell of C96, and click «ascertain». D96 shows «OK», and C23 is $X_{3a}=0.1280$ after Excel finishes the process of trail and error automatically. C97 is η= 13.58 %.

3.2 Amount of solvent needed as X_{3a} is 0.1

Fig. 5 shows the calculating process. Assume S and solve Eqs. 3 simultaneously, find out $X_{3a}^\#$. If $X_{3a}-X_{3a}^\#$ is 0, the assumption is right, unless to operate tool of «seek goal» in Excel till $X_{3a}-X_{3a}^*=0$, and find out S.

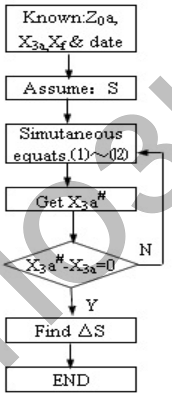
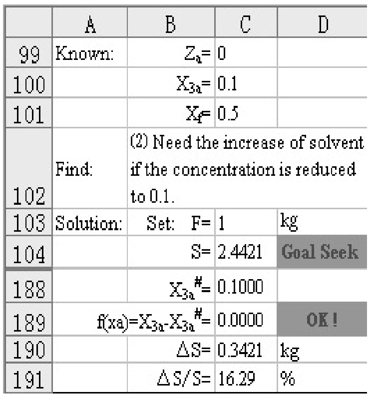


Fig. 5. Schematic of calculation second question



	A	B	C	D
99	Known:	Z_a=	0	
100		X_{3a}=	0.1	
101		X_f=	0.5	
102	Find:	(2) Need the increase of solvent if the concentration is reduced to 0.1.		
103	Solution:	Set: F=	1	kg
104		S=	2.4421	Goal Seek
188		$X_{3a}^\#$=	0.1000	
189		$f(xa)=X_{3a}-X_{3a}^\#$=	0.0000	OK !
190		ΔS=	0.3421	kg
191		ΔS/S=	16.29	%

Fig. 6. Question 2

The main part of this process is similar to 3.1 in detail. The difference of comparison with 3.1 is shown in Fig. 6. Assume S, input initial value of «2.3» in C104, find out C188=0.02356. Operate tool of «goal seek» in Excel, because C188 is not 0, and get S=2.442kg, $X_{3a}^\#=0.1000$, and meet the need of the problem. So get S = 0.3421 kg, S/S=16.29 %.

4 The influence of S/F and Z_a on X_{3a} in the raffinate phase

Influence of the solvent ratio S/F [1.2,2.44] and Z_a [0,0.06] on X_{3a} is shown in Fig.7.

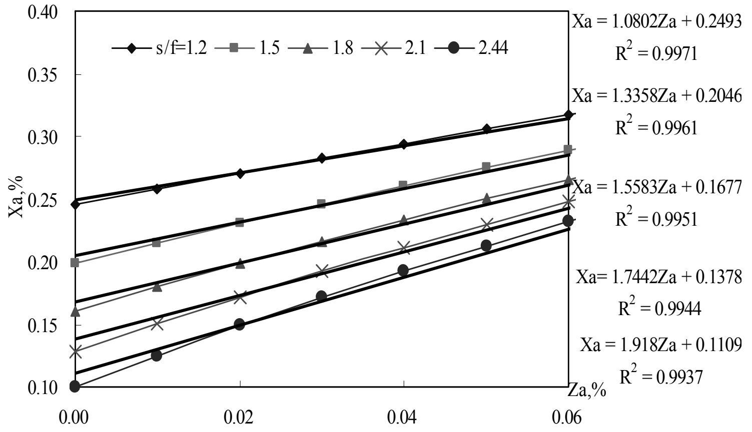


Fig. 7. Influence of Za on Xa at definitive S/F

As can been seen from Fig. 7, X_{3a} changes linearly with Z_a at constant of S/F.So, by RME[6,9]X is $(B^TB)^{-1}B^TY$, and get X_{3a}= 0.3327+1.7269Za-0.0908S/F, R^2=0.972 through regressing. In practice, if X_{3a} decreases, Z_a is a key factor, which belongs to controlling factor. Therefore, Z_a should be first reduced. Next, S/F is appropriately increased. Not only it improves the recovery yield of the product, also reduces the operating costs and increases economic efficiency of company.

5 Conclusions

5.1 Comparison of the results by methods between Excel and constructive

Table shows comparison of the results by methods between Excel and constructive. As shown From Table 1, for the first question, keeping S/F=2.1, X_3a and R_3 in the raffinate phase is 0.1286 and 0.5293 kg actually, rather than 0.15 and 0.775 kg. η is 13.55 %, rather than 22.30 %. Comparing with the analysis method in Excel, the relative errors are 16.64, 46.62 and 64.58 %, respectively; for the second question, X_{3a} = 0.1, S and ΔS is 2.45 kg and 0.342 kg actually rather than 3.0 kg and 0.9 kg, comparing with the analysis method in Excel, the relative error is 22.85 and 163 % respectively.

Table

Comparison calculating results by the two methods

Ques.	Variables	Results		Error, %
		Const.	Excel	
1	X_{3a}	0.1500	0.1286	16.64
	R_3/kg	0.7750	0.5293	46.42
	η/%	22.30	13.55	64.58
2	S/kg	3.0	2.442	22.85
	□S/kg	0.9	0.342	163.1

5.2 The regression equation of water extract acetone–chloroform by countercurrent extraction

Empirical Eq.8 is regressed for acetone in the system of acetone- chloroform is extracted using water with multi-stage countercurrent by RME, and get

$$X_{3a} = 0.3327 + 1.7269\, Z_a - 0.0908S / F.$$

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УДК 66.023

Макрокинетика процесса гидрирования бензола в трубчатых реакторах

Macrokinetics of benzene hydrogenation in a tubular reactor

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Мақалада бензолды гидерлеу процесі даналы катализаторлармен және суытылатын құбырлы реакторда қаралған. Бензолды гидерлеу процесінің макрокинетикасы кәсіп-өндірістік деңгейіне жақындатылған жағдайда зерттелген. Кинетикалық режимінің температурасын және де сыртқы диффузия режимінің сындық температурасын анықтауға мүмкіншілік беретін математикалық формула алынған. Жүйе әр түрлі температура ағымында тұрақты режимге ие болады. Ғылыми зерттеу нәтижелері каталиттік реакцияларды лабораториялық зерттеуден өнеркәсіпке өтуде қолданылуы мүмкін.

In this paper we consider the process of hydrogenation of benzene cooled tubular reactors with a stationary granular bed reactor. Macrokinetics of benzene hydrogenation in tubular reactors under conditions as close as possible to the industry was studied. The mathematical formula for determining the temperature of the kinetic regime as well as the critical temperature external diffusion regime was refered. It was found that at any temperature flow system would have a steady state. The research results can be used in the transition from scale dimension studies of catalytic reactions at the molecular level to the conditions of industrial process implementation.

Реакторы с неподвижным слоем катализатора являются наиболее распространенными системами в области каталитических технологий. Такие реакторы представляют собой неоднородную систему, состоящую из двух фаз: твердых частиц катализатора и промежутков между ними, по которым движется реакционная смесь в виде газа или жидкости [1]. Решение проблем масштабного перехода от лабораторных исследований каталитической реакции на молекулярном уровне до условий промышленной реализации процесса возможно на основе фундаментальных знаний о химических превращениях и физических процессах переноса вещества, тепла и импульса.

Охлаждаемые трубчатые реакторы с неподвижным зернистым слоем катализатора широко используются в химической промышленности для процесса гидрирования бензола [2]. В данной работе этот процесс рассмотрен с условием непористости частиц катализатора. Тогда, считая, что реакция описывается уравнением вида

$$\sum_{i=1}^{N} \nu_i \cdot A_i = 0\,, \tag{1}$$

можно представить стационарный процесс превращения реагентов уравнениями

$$\beta_i \left(c_i - c_{i\infty}\right) = \nu_i \rho\left(c,T\right),\ i = 1,2...N\,; \tag{2}$$

$$\alpha\left(T - T_\infty\right) = h\rho\left(c,T\right). \tag{3}$$