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MATHEMATICAL MODELING OF VINYLACETATA SYNTHESIS REACTOR

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Abstract
In this article impact of different parameters (temperature, volumetric rate, molar ratio of C_2H_2 : CH_3COOH, catalyst preparation method) on the reaction yield of the catalytic acetylation of acetylene was studied. Kinetic model was developed on the basis of results and was optimized vinylacetate synthesis process according the model. Catalyst deactivation was taken into account and mathematical model of ideal substitute for the reactor of vinylacetate synthesis from acetylene and the main parameters of the tube reactor was studied.

Keywords: modeling, acetylene, acetic acid, vinylacetate, catalyst, reactor, volumetric rate, adequacy.

Introduction

In this article impact of different parameters (temperature, volumetric rate, molar ratio of C_2H_2:CH_3COOH, catalyst preparation method) on the reaction yield of the catalytic acetylation of acetylene was studied. Kinetic model was developed on the basis of results and was optimized vinylacetate synthesis process according the model. Catalyst deactivation was taken into account and mathematical model of ideal

substitute for the reactor of vinylacetate synthesis from acetylene and the main parameters of the tube reactor was studied.

Annual demand for vinylacetate in worldwide is 5 million tons and in the Republic of Uzbekistan is 30000 tons. Currently vinylacetilene has been produced in Eastern and Western Europe and Asia [1-5]. Several developed countries produce vinylacetate in two methods:

1) Ethylene oxidative etherification (the Moiseev reaction). The process takes place in the presence of ethylene, acetic acid and water.

$$C_2H_4 + CH_3COOH + \frac{1}{2}O_2 \rightarrow CH_2 = CHOCOCH_3 + H_2O$$

2) The catalytic reaction of acetylene and acetic acid in steam phase:

$$C_2H_2 + CH_3COOH \rightarrow CH_2 = CHOCOCH_3$$

The first method is popular because of the low cost of ethylene than acetylene. Nowadays cheap method of acetylene production as a byproduct of new production processes. For this reason it is actual studying of the reaction the production of vinylacetate from acetylene, modeling and optimization of the process reactor [6-11].

Experimental

Many processes technology is related to the activity of the catalyst. Activity and selectivity of the catalyst determines the rate of reaction and qualitative proceeding. Vinylacetate synthesis from acetylene and acetic acid in presence of stationary layered catalyst was carried out in a tube reactor. Taking into account of the catalyst deactivation, `mathematical model of the ideal substitutional reactor for vinylacetate synthesis from acetylene and acetic acid may be described as:

$$\frac{\partial x}{\partial l} = \frac{\Theta(v+1)}{v(volumetric)} \mathrm{r(m, V_{volumetric}}, T, x);$$

$$\frac{\partial \Theta}{\partial t} = \Theta k_p \quad (T)$$

Approximation conditions:

$$x(0,t) = 0; \quad t \in [0, t_k]; \qquad \Theta(\ell, 0) = \Theta_0; \quad \ell \in [0, \ell_p]$$

where V-volume ratio of acetylene and acetic acid; v(volumetric) volumetric rate of raw materials; t-impact time of the catalyst; Θ-variable describing the catalytic activity change; T-temperature ($T \leq 180^0 C$); ℓ_p-length of the reactor; t_k-working time of the catalyst [12-13].

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Results and Discussion

Calculation results of vinylacetate production in tube reactor main working parameters were determined (Tab. 1).

Table 1.
Main parameters of vinylacetate production in tube reactor

T, °C	P, MPa	$U_{g \cdot p \cdot mg}$, m/s	Heat carrier	G, thousand tons/year	D, m	h, m	N, min piece
170-200	0.1	0.60	Boiled water	50	2.5	6.5	4.7

Optimization of vinylacetate synthesis process.

Vinylacetate synthesis yield from acetylene is depend on 3 parameters: process temperature (x_1), volumetric rate of acetylene, and height of catalyst layer (x_3).

Preliminary experimental series according to 2^3 complete factor `experiment plan were carried out. Complete factor experimental plan-matrix and its results is given in Tab. 2.

Following polynomial was taken from the treatment of experimental results: $Y = 21 + 8x_1 - 16x_2 + 10x_1x_1$. In order to analytical optimization of the model, one have to take the model as an incomplete quadratic equation, and solving the optimization make two linear equations:

$$\partial y / \partial x_1 = 8 + 10x_2 = 0 \rightarrow x_2 = -\frac{8}{10} = -0{,}8$$

$$\partial y / \partial x_2 = 16 + 10x_1 = 0 \rightarrow x_2 = -16/10 = -1{,}6$$

Then the optimized equation becomes:

$$Y_{x_2=0,8} = 21 + 8x_1 - 16 \cdot 0{,}8 + 10x_1 \cdot 0{,}8 = 8{,}2 + 16x_1$$

Vinylactetate synthesis from acetylene and acetic acid takes place on $(ZnO)_x \cdot (CdO)_y \cdot (ZrO_2)_z$ catalyst. Adding ZrO_2 to the catalyst deceases the formation of byproducts and also prevents formation of resin in the pores of the catalyst, causing increase the working time of catalyst.

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Table 2. Complete factor experimental plan-matrix and its results is given

Factor degrees and changing range		x_1	x_2	x_3	
0th degree $(x_i = 0)$		185	280	40	
Change range (Δx_i)		25	50	10	
Low degree $(x_i = -1)$		160	230	30	
High degree $(x_i = +1)$		210	330	50	
	Plan	x_1	x_2	x_3	Y
Experiments	1	-	-	-	20.5
	2	+	-	-	28.3
	3	-	+	-	26.8
	4	+	+	-	34.6
	5	-	-	+	26.4
	6	+	-	+	44.2
	7	-	+	+	52.7
	8	+	+	+	70.5

Conclusions

Different factors (volumetric rate, molar ratio of C_2H_2:CH_3COOH, catalyst preparation method) effect on the catalytic acetylation of acetylene were studied. Kinetic model was developed based on the results and optimization carried out according the equation. Taking into account of the catalyst deactivation, the mathematical model for the substitutional reactor for vinylacetate synthesis from acetylene and acetic acid was developed and main parameters of tube reactor was determined.

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