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ENGINEERING PROBLEMS. OPERATION AND PRODUCTION

Mathematical Modeling of the Dehydrating Ethanol to Ethylene Process in a Multitubular Reactor on a Ring-Shaped Alumina Catalyst

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Abstract—The process of dehydrating ethanol to ethylene by varying geometrical dimensions of a ring-shaped alumina catalyst is studied using a mathematical 2D model of a multitubular reactor. The set of ring sizes determines equivalent grain size R_{eq}, on which catalyst's effectiveness factor η depends in turn. A procedure is proposed for assigning grains with different geometric dimensions to four structural groups, depending on the technique used to synthesize samples with the same equivalent size R_{eq}. Based on this approach, a system of criteria is developed for selecting catalyst grains with the best characteristics for given conditions. The geometric sizes of grains and other parameters that ensure the highest ethylene yield at the lowest values of the pressure drop and the residence time are determined.

Keywords: mathematical model, multitubular reactor, dehydrating ethanol to ethylene, alumina catalyst, ring, catalyst's effectiveness factor, equivalent grain size, pressure drop

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INTRODUCTION

Mathematical modeling is commonly used for processes in catalytic reactors in order to solve problems of modernizing existing plants and develop new technological processes. Mathematical modeling enables us to predict the character of a process in different structural elements of process flowsheets and serves as a major tool when analyzing the effect of kinetic, physicochemical, hydrodynamic, and other factors on process parameters [1–8]. Its use also reduces the required number of full-scale experiments considerably and simplifies scaling up.

The catalytic dehydrating of bioethanol derived from different types of edible and inedible feedstocks to ethylene is one of the most advanced contemporary trends in green chemistry [9–15]. In [15], the ethanol dehydrating process on a trefoil-shaped catalyst with equivalent radius $R_{eq} = 0.28$ mm was studied experimentally in the multitubular reactor of a pilot plant. Studies were performed on an acid-modified alumina catalyst [16, 17] prepared by thermal activation of hydrargillite in a TSEFLAR^{TM} reactor [18]. The small size of this catalyst and the relatively high effectiveness factor ($\eta = 0.79$) led to high conversion of ethanol ($X = 94$–98%) at a weight hourly space velocity of 4–6 h^{-1} for 94.5% ethanol, but this was attained with increased pressure drop of the catalyst bed (up to $\Delta P = 0.07$ bar). Using catalyst grains with a greater equivalent pore channel diameter (particularly ring-shaped grains) lowers ΔP [7, 19]. In addition, ring-shaped grains are very simple to manufacture and are widely used in various catalytic processes.

In-depth analysis and searching for the optimum conditions of the ethylene from bioethanol processing on catalysts of various natures with allowance for the specific features of different catalytic reactors is a theoretical problem that has not been solved sufficiently. In particular, it is necessary to study the effect of the shapes and sizes of catalyst grains on the ethanol to ethylene dehydrating in a multitubular reactor [14, 15]. Considerable temperature gradients across the tube radius exist even at moderate heat fluxes. Hence, the use of 2D mathematical models that include descriptions of the processes of heat and mass transfer in the axial and radial directions is required. Quasi-homogeneous 2D mathematical models have shown good results in studying, predicting, and calculating heterogeneous catalytic processes in multitubular reactors [1, 2, 4, 7, 14, 20, 21]. In such models, the catalyst and the flowing gas are presented as a continuous quasi-homogeneous medium, while the mass and heat fluxes are described by differential equations of heat and mass transfer.

The catalytic process of dehydrating ethanol to ethylene in a multitubular reactor is characterized by high parametric sensitivity to temperature. The tube's diameter and the shape and size of the catalyst grains determine the efficiency and parametric sensitivity of

this process. The geometric characteristics of the grains affect the effectiveness factor η, the effective bed heat conductivity, the intensity of radial and axial heat and mass transfer in a fixed catalyst bed, and pressure drop ΔP of the catalyst bed. Compared to spherical or cylindrical grains, ring-shaped catalysts and catalysts with more sophisticated geometric shapes have more developed surfaces of contact with the gas phase, lower bulk density γ_b (and therefore create high bed porosity), and a smaller equivalent radius R_{eq}. The last factor plays an important role in diffusion mass transfer inside grains, since it ensures higher values of η and observed reaction rates and thus increases the activity per unit catalyst bed volume.

The aim of this work was to study by mathematical modeling the effect of the size of a ring-shaped catalyst on the performance of the process of ethanol dehydrating in a multitubular reactor. We solved the problem of estimating the geometric sizes of catalyst grains, which contribute to ΔP reduction when ethanol conversion is reached as higher as 98% under given process conditions.

MATHEMATICAL MODEL AND CONDITIONS OF CALCULATION

The mathematical modeling of a catalytic process in a multitubular reactor with a fixed granular bed was done using a quasi-homogeneous 2D model. Our mathematical model [7, 14] was a system of differential material and heat balance equations and considered a number of physical and chemical factors: (1) the chemical conversion of reagents in the form of kinetic equations for the rates of the reactions that occur in the process of dehydrating ethanol to ethylene; (2) the process of transfer inside a porous catalyst grain in the form of diffusion and heat conductivity equations for a grain; (3) the transfer of heat along the tube's radius through heat conductivity and the transfer of heat and mass along the tube's length through convection; (4) the change in the linear gas velocity due to reactions that occur upon a change in volume and a change in temperature and pressure along the catalyst bed.

The kinetic model of the catalytic process of ethanol dehydrating on alumina catalysts [14] considers the reactions of the formation of ethylene (C2) from ethanol (E) and diethyl ester (DEE) and the formation of such byproducts as acetaldehyde (AA) and butylene (C4). The corresponding reaction rates are described by semiempirical equations in the form of power functions:

$$C_2H_5OH \rightarrow C_2H_4 + H_2O \qquad r_1 = k_1P_E,$$

$$C_2H_5OH \rightarrow 0.5\ C_2H_5OC_2H_5 + 0.5\ H_2O \qquad r_2 = k_2P_E^2,$$

$$C_2H_5OC_2H_5 \rightarrow 2\ C_2H_4 + H_2O \qquad r_3 = k_3P_{DEE},$$

$$C_2H_5OH \rightarrow C_2H_4O + H_2 \qquad r_4 = k_4P_E,$$

$$C_2H_4 \rightarrow 0.5\ C_4H_8 \qquad r_5 = k_5P_{C2}^2,$$

where P_i is the partial pressures of reaction mixture components; k_j is a kinetic constant; r_j is the rate of the j-th reaction; $W_i = \sum \nu_{ij} r_j$ is the rate of the formation of the i-th product in the j-th reaction; and ν_{ij} is the stoichiometric coefficient of the i-th component in the j-th reaction.

The above mathematical model with the given kinetic equations satisfactorily describes the catalytic process of ethanol dehydrating in a multitubular reactor on an alumina catalyst [14] and enables us to calculate the distribution of temperatures and concentrations of reaction mixture components along the radius and length of the catalyst bed.

The parameters used as the main performance characteristics for the catalytic process in a multitubular reactor were ethanol conversion X, selectivity to products S_i, ethylene yield Y, and residence time on weight basis τ_G. The formulas for calculating these parameters are

$$X = 100\frac{C_E^0 - \Delta V C_E^k}{C_E^0}, \quad S_i = 100\frac{\frac{1}{\nu_i}C_i^k}{\sum\frac{1}{\nu_i}C_i^k},$$

$$Y_{C2} = XS_{C2}, \quad \tau_G = 3600\frac{G_{CAT}}{W_E},$$

where C_E^0 and C_E^k are the ethanol concentration at the reactor inlet and outlet, mol. fractions; ΔV is the coefficient of the change in the reaction mixture volume; C_i^k is the concentration of reaction products at the reactor outlet, mol. fractions; ν_i is the stoichiometric coefficients; G_{CAT} is the catalyst mass, kg; and W_E is the 94.5 wt % ethanol mass flow rate, kg/h.

The Thiele number characterizing the value of η was determined by calculating equivalent grain size R_{eq} as the ratio of the geometric volume of a grain to its geometric surface area. The effective diffusion coefficient includes the Knudsen and molecular diffusion coefficients and a correction expressed as a semiempirical permeability coefficient that considers the shape, porosity, roughness, and tortuosity of the porous grain structure [22]. The coefficient of molecular diffusion was calculated for a multicomponent ethylene–ethanol–diethyl ester–water–nitrogen mixture according to Wilke [23]. Specific pressure drop $\Delta P/L$ of the granular bed was calculated using formulas for grains with sophisticated shapes [7, 19].

In calculating the process of dehydrating ethanol to ethylene in a multitubular reactor, our constant parameters were the composition of the initial vapor–gas mixture (mol %) [E] : [H_2O] = 87.05 : 12.9; inner tube diameter d_T = 27.3 mm; linear gas velocity U = 0.65 m/s; and heat agent temperature T_W = 420°C. Our varied parameters were catalyst bed height L and such dimensions of the catalyst grains as outer diame-

ter D_{OUT} = 4–9 mm, inner diameter D_{IN} = 2–7 mm, and height h = 1.3–7 mm.

The catalyst samples for our theoretical studies were first selected according to the results from estimating the effect of the ring size on η and ΔP. The best catalyst samples were then determined by the mathematical modeling of the process on the selected catalyst samples under the same conditions at a fixed value of ethanol conversion. A trefoil-shaped catalyst with above characteristics R_{eq} and η (below, 0R28) was considered the reference sample in this work.

The parameters of the process regimes, the characteristics of the alumina ethanol dehydrating catalyst, and the first-order reaction rate constants used to calculate η were taken from [15]. In analyzing the effect of the catalyst grain size, we considered the possibility of their practical fabrication, including the plasticity of molded masses of aluminum hydroxide intended for extrusion and the mechanical strength of the resulting granules [24]. For convenience, the process parameters obtained on ring-shaped catalyst grains were normalized to those obtained under the same conditions on reference sample 0R28.

PRELIMINARY SELECTION OF GRAINS

The effect of the equivalent radius R_{eq} on the effectiveness factor η and specific pressure drop $\Delta P/L$ of the catalyst bed was estimated to select catalyst samples for the preliminary mathematical modeling of the process in a multitubular reactor. Values of the characteristics η, $\Delta P/L$ and bulk catalyst density γ_b for ring-shaped grains were normalized to the same parameters of trefoil-shaped grains (0R28).

The normalized values of η on ring- and trefoil-shaped grains with the same equivalent size R_{eq} of 0.28 mm were close to 1, but raising R_{eq} to more than 0.43 mm appreciably reduced η by more than 30% with respect to 0R28 (Fig. 1). The reducing in η suggests the process on a grain shifts from the kinetic- to the diffusion-controlled region, thus lowering the observed reaction rate. It is therefore inadvisable to raise R_{eq} to more than 0.43 mm. Variants of the geometric ring characteristics with allowance their accepted limitations are given in Table 1.

The ring dimensions were determined by varying the ring wall thickness δ, the inner diameter D_{IN}, the outer diameter D_{OUT}, and the ring height h at a fixed value of one of these parameters (see Table 1).

The dependences of normalized parameters η, γ_b, and $\Delta P/L$ on equivalent radius R_{eq} for samples of groups I–IV are plotted in Fig. 1. In groups II and III, the equivalent radius was varied mainly by changing wall thickness δ, while outer diameter D_{OUT} changed only slightly (see Table 1). This change in sizes had a considerable effect on parameters η and γ_b, but had virtually no effect on the specific pressure drop $\Delta P/L$

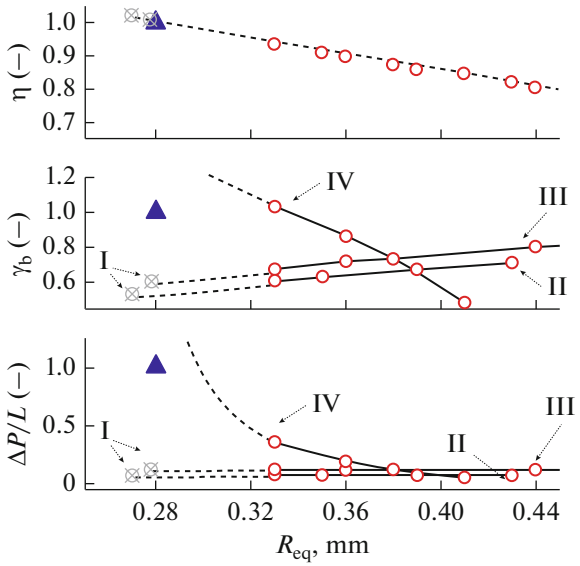

Fig. 1. Normalized effectiveness factor η, catalyst bulk density γ_b, and pressure drop $\Delta P/L$ versus catalyst grain size R_{eq}. I–IV are the groups of catalyst samples in Table 1. (○) Rings, (⊗) rings of group I, and (▲) trefoil 0R28.

of the bed. In group IV (at fixed wall thickness δ and varied D_{IN} and D_{OUT}), parameters η, γ_b, and $\Delta P/L$ fell as R_{eq} rose. Parameter $\Delta P/L$ on the samples of this group with equivalent sizes of less than 0.38–0.39 mm

Table 1. Geometric characteristics of ring*

Catalyst samples		Ring size, mm			D_{IN}, mm	R_{eq}, mm
		D_{OUT}	h	δ		
IR27	I group	5.2	5.20	0.60	4.0	0.27
IR28		5.4	2.70	0.70	4.0	0.28
IR28		2.5	1.25	1.00	0.5	0.28
IIR33	II group	5.5	5.50	0.75	4	0.33
IIR35		5.6	5.60	0.80		0.35
IIR39		5.8	5.80	0.90		0.39
IIR43		6.0	6.00	1.00		0.43
IIIR33	III group	5.7	2.85	0.85	4	0.33
IIIR36		5.9	2.95	0.95		0.36
IIIR38		6.0	3.00	1.00		0.38
IIIR44		6.4	3.20	1.20		0.44
IVR33	IV group	4.0	2.00	1	2	0.33
IVR36		5.0	2.50		3	0.36
IVR38		6.0	3.00		4	0.38

* D_{OUT} is the outer diameter, D_{IN} is the inner diameter, h is the height, and δ is the wall thickness.

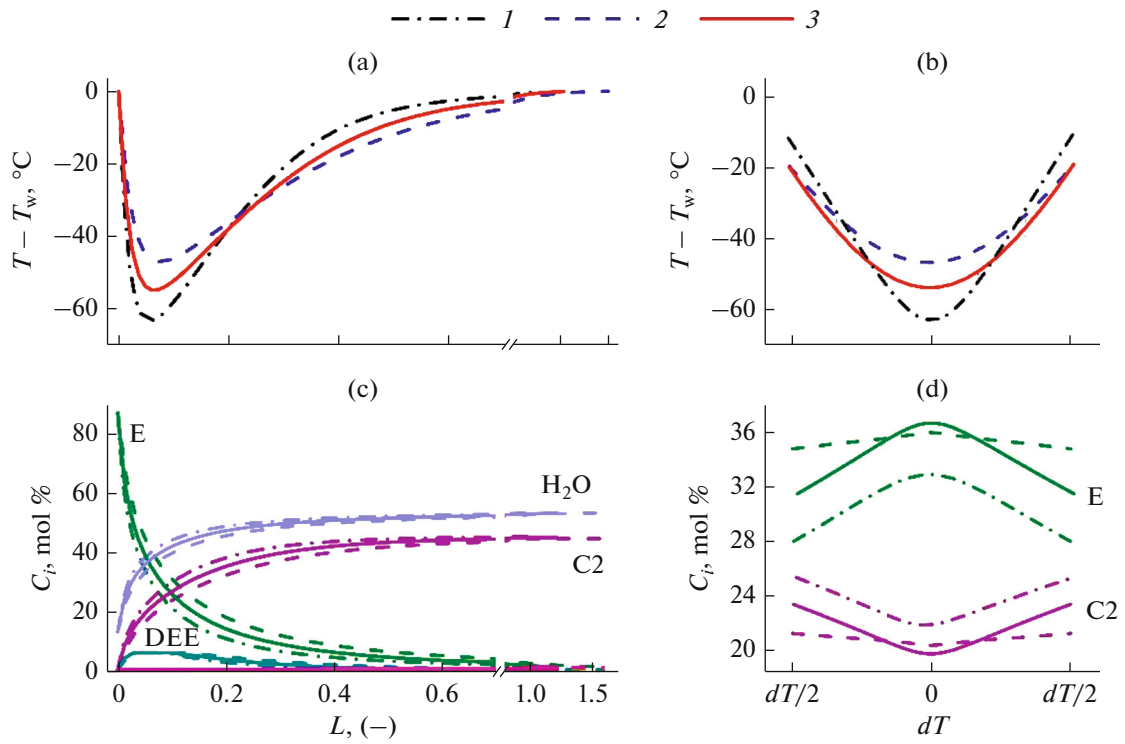

Fig. 2. (a, c) Axial and (b, d) radial profiles of temperature and concentration in a multitubular reactor for grains shaped as (*1*) trefoil of 0R28 and rings (*2*) IIR43 and (*3*) IIIR33. $T - Tw$ is the difference between the reactor and heat transfer fluid temperatures.

was higher than on the rings of groups II and III, but ~3 times lower (for IVR33–IVR38) than on the trefoil-shaped reference catalyst.

Alumina ring-shaped catalyst grains with wall thicknesses δ of less than 0.8 mm or heights h of less than $0.5D_{OUT}$ have insufficient mechanical strength and are not used in practice. Such rings with equivalent sizes of 0.28–0.27 mm were combined into separate group I. Modern catalyst molding allows us to obtain ring-shaped catalyst grains with equivalent size R_{eq} of no less than 0.33 mm. We may therefore assume that grains IIIR33, IVR33, and IIR35 with equivalent sizes of 0.33–0.35 mm are the smallest of the grains available in practice. They ensure a high observable reaction rate due to moderate inner diffusion resistance and simultaneously have sufficient mechanical strength and low pressure drop for use in a multitubular reactor.

Mathematical modeling of the ethanol dehydrating process in a multitubular reactor was done using the samples listed in Table 1.

COMPARATIVE ANALYSIS OF THE PROCESS ON CATALYSTS OF VARIOUS DIMENSIONS AT THE CONSTANT ETHANOL CONVERSION

Our comparative study of process performance characteristics on ring-shaped catalysts with different grain sizes was performed at the same initial process parameters by varying the value of τ_G required to attain the ethanol conversion $X = 98\%$. The process parameters obtained on ring-shaped catalyst grains were subsequently normalized to those obtained on reference sample 0R28.

The calculated axial and radial concentration and temperature profiles in beds of catalyst rings of various dimensions are plotted in Fig. 2. Compared to sample 0R28, the temperature and reagent concentration profiles in the bed of ring-shaped grains are smoother in both the axial and radial directions, and the temperatures in the reactor are nearly 12°C higher on average. The rise in temperature in the bed of rings can be explained by lower activity per unit bed volume (due to higher porosity), which also results in a slower rate of heat absorption for endothermic reactions. The effect of a rise in reactor temperature can be either positive (with increased activity and a shorter residence time needed to achieve the specified conversion) or negative (with an increase in the selectivity toward byproducts).

The selectivities toward target products and byproducts are given in Table 2 for the selected rings and sample 0R28, and the dependence of the selectivity on the ethanol conversion in a multitubular reactor is plotted for some grains in Fig. 3. The selectivity toward products on rings differs negligibly, so the difference can be seen only for C4 in Fig. 3. The selectivity toward byproducts on rings is higher and grows along with R_{eq} (see Table 2). The selectivity toward the intermediate product (DEE) at the same conversion

was 0.040 ± 0.003 mol % for all samples (Table 2). The selectivity toward ethylene reaches maximum value of 97.5–98% at the ethanol conversion of 94–96%. (see Fig. 3). However, it falls when the degree of conversion rises to 98%, due to the reaction of ethylene dimerization with the formation of butylene. However, ethylene yield Y continues to grow even at degrees of conversion higher than 94–96% (see Fig. 3).

The dependence of the process performance characteristics in a multitubular reactor on the size of rings is shown in Fig. 4. Compared to sample 0R28, the ethylene yield is slightly lower on all of the rings, but the required catalyst bed height is greater. The residence time and the pressure drop are proportional to the bed's porosity and correspond to the earlier demonstrated character of the change in parameter γ_b, which was different for the samples of groups II, III, and IV. The residence time τ_G for the samples with equivalent sizes of 0.37–0.40 mm is comparable to that of the reference sample. The pressure drop on all rings except IVR33–IVR36 is ~2 times lower, which plays an important role in the choice of a catalyst.

The height of a ring-shaped catalyst needed to achieve $X = 98\%$ is 1.2–1.7 times greater than for sample 0R28, generally due to lower η and higher bed porosity (see Fig. 4b). In terms of the residence time τ_G, these differences are ±20% upon a ±15% change in R_{eq} for groups II and III, relative to grains with R_{eq} = 0.37–0.40 mm (see Fig. 4c).

When the equivalent size of grains grows, the required residence time τ_G increases, due to a decrease in the rates of catalytic ethanol dehydrating as a result of stronger diffusion resistance. An increased residence time and an elevated reactor temperature can lead to greater selectivity toward byproduct butylene (see Table 2), thereby reducing the yield of the target product (ethylene) (see Fig. 4a). The lowest ethylene yield is observed for grains IIR43 and IIIR44, which have the greatest size.

Independently of the way of varying the geometric dimensions of rings at constant values of equivalent radius R_{eq} in groups I–IV (see Table 1), the ethylene yield (see Fig. 4a) and the bed height (see Fig. 4b) changed slightly, within ≈0.03% and ≈7 rel %, respectively. Maximum yield Y at a bed height L close to its minimum value was achieved on the smallest grain of group III. The difference between the residence time τ_G (see Fig. 4c) and the pressure drop (see Fig. 4d) was greater. The grain wall thickness was varied in groups II and III. The pressure drop ΔP obtained on the grains of group II ($h = 1D_{OUT}$) was lower, and the required residence time τ_G was nearly 6–9% smaller than with group III ($h = 0.5D_{OUT}$). In group IV, where D_{IN} was varied at fixed wall thickness δ = 1 mm and $h = 0.5D_{OUT}$, grains with equivalent radii of 0.37–0.40 mm provide acceptable activity and pressure drop values only within a very narrow range of geometric dimensions (D_{OUT} = 5.5–6.0 mm, h = 2.75–3.0 mm, D_{IN} = 3.8–4.0 mm).

Table 2. Selectivities to the ethanol dehydrating products in a multitubular reactor on ring-shaped catalysts

Catalyst*	Selectivity, mol %		
	$S_{C2} + S_{DEE}$	S_{AA}	S_{C4}
0R28	97.59	0.20	2.27
IR28	97.19	0.21	2.60
IIR33	96.78	0.22	3.00
IIR35	96.61	0.22	3.16
IIR39	96.28	0.23	3.49
IIR43	95.95	0.24	3.81
IIIR33	96.80	0.22	2.97
IIIR36	96.53	0.23	3.24
IIIR38	96.40	0.23	3.37
IVR33	96.75	0.22	3.03
IVR36	96.54	0.23	3.23
IVR38	96.40	0.23	3.37

*For sample denotation, see Table 1.

In general, grains R33–R43 of groups II and III ensured acceptably high values for ethylene yield Y at sufficiently low ΔP and τ_G. The best combination of the highest ethylene yield, the shortest residence time, and the lowest pressure drop was obtained for grain IIR33 with the smallest size. Using catalysts shaped as rings with equivalent sizes of 0.33–0.43 mm, we can therefore achieve an ethylene yield Y comparable to the one obtained on reference sample 0R28, but at much lower ΔP. For practical use, we can recommend rings with certain geometric dimensions: outer diameter D_{OUT} = 5.6–6.0 mm, ring height h = 2.85–6.0 mm, inner diameter D_{IN} = 3.8–4.0 mm

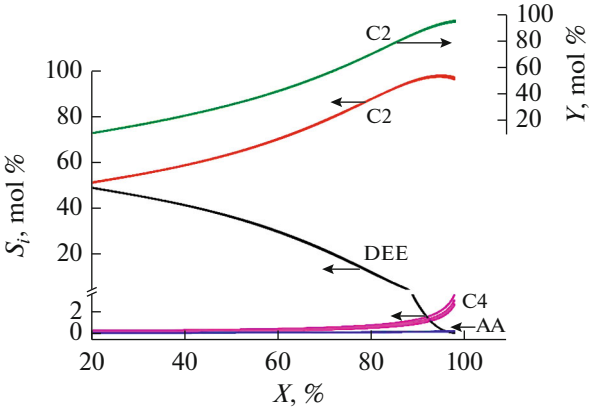

Fig. 3. Ethylene yield Y and selectivity toward products S versus ethanol conversion X for ring-shaped grains IIR39, IIR35, and IIIR33 in a multitubular reactor.

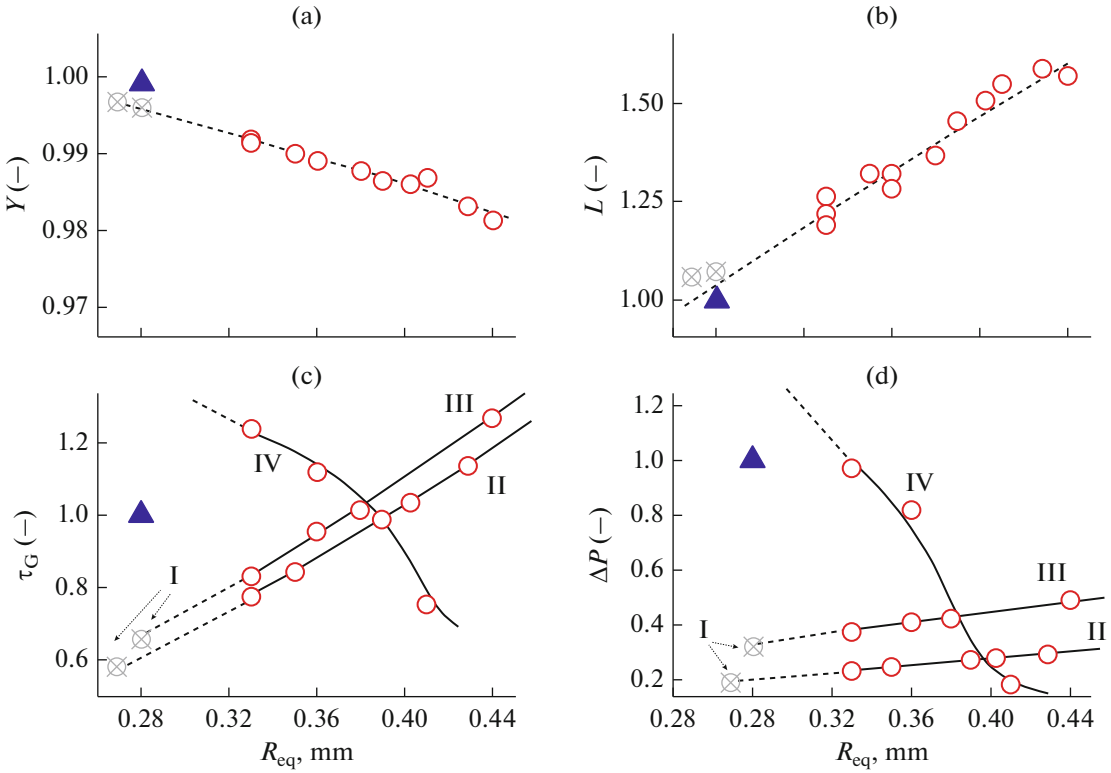

Fig. 4. Comparison of normalized performance characteristics for the process in a multitubular reactor on (▲) grains with the trefoil shape of 0R28, (○) rings, and (⊗) rings of group I at varied R_{eq} for the catalysts of groups I–IV (see Table 1): (a) ethylene yield, (b) catalyst bed height, (c) residence time, (d) pressure drop.

CONCLUSIONS

Numerical analysis of the catalytic process of dehydrating ethanol to ethylene in a multitubular reactor on ring-shaped catalyst grains was performed using a 2D mathematical model. A procedure was proposed for assigning grains with different geometric dimensions to four structural groups, depending on the way used to design grains with the identical equivalent size. Based on this approach, a two-stage system of criteria was developed for selecting catalyst grains with the best performance characteristics under specified conditions. They were selected mainly by comparing the effectiveness factor and the pressure drop per unit bed length. A comparative analysis of the process parameters on catalysts of different sizes was performed at the same degree of ethanol conversion.

The dependences of the main technological characteristics of the process in a multitubular reactor (e.g., pressure drop ΔP of the catalyst bed, molar ethylene yield Y, and residence time τ_G required to achieve the ethanol conversion X = 98%) on the equivalent size of a catalyst grain were studied.

As a result of modeling, we determined the geometric dimensions of grains and other parameters that ensured the highest ethylene yield at an ethanol conversion of 98% and the lowest pressure drop and shortest residence time. It was established that ring-shaped catalysts with equivalent radii of 0.33–0.43 mm satisfy such criteria. Considering the technical capabilities of design, rings with the following sizes: outer diameters of 5.6–6, heights of 2.85–6, and wall thicknesses of 0.8–1 mm, can be recommended for the ethanol to ethylene dehydrating process in a multitubular reactor.

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