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RESEARCH ARTICLE

Modeling of the synthesis of mono-, di-, tri- and tetraesters by catalytic esterification of pentaerythritol with carboxylic acids C_4–C_{10} under polar solvent conditions

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Abstract

Objectives. The study set out to establish the scientific basis for the catalytic esterification of aliphatic carboxylic acids C_4–C_{10} with pentaerythritol in a polar solvent, sulfolane. The kinetic parameters of the forward and reverse reactions were determined along with the influence of the carboxylic acid structure on the rate of conversion and the component composition of the reaction products.

Methods. The process was carried out in a perfectly stirred tank reactor with an excess of carboxylic acid (the molar ratio of pentaerythritol to carboxylic acid was 1 to 8, respectively) in a temperature range of 383.2–403.2 K. A combination of sulfolane and methanesulfonic acid was used as a catalytic system. This combination, which was found to be more effective as compared to the self-catalytic process, manifested in a 600–800-fold increase in the reaction rate at optimal amounts of sulfolane (30% by weight of the reaction system) and methanesulfonic acid (1% by weight of the reaction substrate). The composition of the reaction products was monitored by gas–liquid chromatography with preliminary calibration using pure substances. Chromatographic analysis was performed using a Kristall 2000M chromatograph equipped with a capillary column (60 m × 0.32 mm × 0.5 μm) with a grafted stationary phase BP-1 (100% dimethylpolysiloxane).

Results. For the first time, the parameters of the Arrhenius equation for the forward and reverse reactions of the esterification of 14 aliphatic carboxylic acids C_4–C_{10} of various structures with pentaerythritol in a sulfolane medium were obtained. The resulting kinetic models satisfactorily describe the experimental data as confirmed by standard statistical calculation methods (in our case, the Pearson test was chosen, which is sensitive to a sufficiently large array of experimental data; the test value was at least 96%, indicating the adequacy of the kinetic model used to describe the processes). The influence of the carboxylic acid structure on the process rate and the composition of the reaction products was evaluated.

Conclusions. The conducted studies revealed that the composition of reaction products under chemical equilibrium conditions under the selected conditions is virtually independent of the structure of the carboxylic acid: the chemical reaction rate is determined primarily by the structure of the carboxylic acid. The obtained data can be used to substantiate verified kinetic models that provide the possibility of rational design of the synthesis of target esters with a high degree of selectivity and predictable properties.

Keywords

pentaerythritol esters, activation energy, pre-exponential factor, kinetic control, sulfolane

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НАУЧНАЯ СТАТЬЯ

Моделирование синтеза моно-, ди-, три- и тетраэфиров каталитической этерификацией пентаэритрита карбоновыми кислотами C_4–C_{10} в среде полярного растворителя

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Аннотация

Цели. Изучение научных основ каталитической этерификации алифатических карбоновых кислот C_4–C_{10} пентаэритритом в среде полярного растворителя — сульфолана. Определение кинетических параметров процесса прямых и обратных реакций. Оценка влияния структуры карбоновой кислоты на скорость превращения и компонентный состав продуктов реакции.

Методы. Процесс проводили в реакторе идеального смешения в избытке карбоновой кислоты (мольное соотношение пентаэритрита к карбоновой кислоте составляло 1 к 8 соответственно), в температурном интервале 383.2–403.2 К, в качестве каталитической системы использовали сочетание сульфолана и метансульфокислоты; данное сочетание показало свою эффективность по сравнению с проведением процесса в режиме самокатализа, что проявляется в увеличении скорости реакции в 600–800 раз при оптимальных количествах сульфолана (30 мас. % от реакционной системы) и метансульфокислоты (1 мас. % от реакционного субстрата). Контроль состава продуктов реакции осуществляли методом газожидкостной хроматографии с предварительной калибровкой по чистым веществам. Хроматографический анализ проводили на базе хроматографа «Кристалл-2000М», оснащенного капиллярной колонкой (60 м × 0.32 мм × 0.5 мкм) с привитой неподвижной фазой BP-1 (100% диметилполисилоксан).

Результаты. Впервые получены параметры уравнения Аррениуса для прямых и обратных реакций процесса этерификации 14 алифатических карбоновых кислот C_4–C_{10} различного строения пентаэритритом в среде сульфолана. Полученные кинетические модели удовлетворительно описывают экспериментальные данные, что подтверждено стандартными статистическими методами расчета (в нашем случае избран критерий Пирсона, который является чувствительным к достаточно большому массиву экспериментальных данных; значение критерия составляло не менее 96%, что говорит об адекватности используемой кинетической модели для описания протекающих процессов). Дана оценка влияния структуры карбоновой кислоты на скорость процесса и состав продуктов реакции.

Выводы. В результате проведенных исследований установлено, что состав продуктов реакций в условиях химического равновесия при избранных условиях практически не зависит от структуры карбоновой кислоты; скорость химической реакции определяется, в основном, структурой карбоновой кислоты. Полученные данные позволяют аргументировать верифицированные кинетические модели, обеспечивающие возможность проектирования синтеза целевых эфиров с высокой степенью селективности и предсказуемыми свойствами.

Ключевые слова

сложные эфиры пентаэритрита, энергия активации, предэкспоненциальный множитель, кинетический контроль, сульфолан

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INTRODUCTION

Pentaerythritol esters constitute an important class of multifunctional organic compounds obtained by the esterification of pentaerythritol with monobasic carboxylic acids. By varying the degree of substitution of hydroxyl groups in the pentaerythritol molecule (from mono- to tetraesters), substances with a wide range of properties can be obtained. These are used in various industries, from fifth-generation synthetic lubricants and plasticizers to components of paint and varnish coatings, cosmetics, and functional additives in the food and pharmaceutical industries [1–3].

Pentaerythritol tetraesters are of particular interest in a number of technical fields. This group of esters is characterized by high thermal stability, low volatility, and satisfactory rheological properties, particularly in the context of lubricants and high-temperature technical fluids [4–7]. Mono-, di-, and triesters are also of significant value, serving as intermediates in multistep syntheses as well as standalone substances used in the production of solvents, emulsifiers, biodegradable surfactants, including as structural units in the synthesis of polyesters and polymeric materials with specified properties [8–10].

The synthesis of pentaerythritol esters proceeds in a stepwise manner (see diagram). The theoretical basis for the formation of intermediate products has not been sufficiently studied. Most available studies focus on obtaining the final product—tetraester—without providing a systematic analysis of the preceding stages and their mutual influence [11–13]. This significantly limits possibilities for targeted control of the process selectivity and the development of energy-efficient synthesis conditions.

The aim of this study is to research the scientific fundamentals and model the sequential esterification of pentaerythritol with aliphatic carboxylic acids having a carbon chain length of C_4–C_{10} in the presence of methanesulfonic acid as a catalyst and sulfolane as a polar high-temperature solvent, the effectiveness of which we have previously demonstrated [14].

MATERIALS AND METHODS

Reagents

The following reagents were used in the experiment: *n*-pentanoic acid (**1**, 99%, *Sigma-Aldrich*, USA); *n*-hexanoic acid (**2**, 98%, *Pallav Chemicals*, India); *n*-heptanoic acid (**3**, 98%, *Acros Organics*, USA); *n*-octanoic acid (**4**, 99%, *Sigma-Aldrich*, USA); *n*-nonanoic acid (**5**, 99%, *Sigma-Aldrich*, USA); *n*-decanoic acid (**6**, 99%, *Sigma-Aldrich*, USA); isobutanoic acid (**7**, 99%, *Sigma-Aldrich*, USA); isopentanoic acid (**8**, 99%, *Sigma-Aldrich*, USA); 2,2-dimethylpropanoic acid (**9**, 99%, *Sigma-Aldrich*, USA); 2-methylpentanoic acid (**10**, 98%, *Merck*, Germany); 4-methylpentanoic acid (**11**, 99%, *Sigma-Aldrich*, USA); 2,2-dimethylbutanoic acid (**12**, 98%, *Acros Organics*, USA); 2-ethylbutanoic acid (**13**, 99%, *Acros Organics*, USA); 2-ethylhexanoic acid (**14**, 95%, *SIBUR*, Russia); pentaerythritol (95%, *METAFRAX CHEMICALS*, Russia); methanesulfonic acid (70%, aqueous solution, *Acros Organics*, USA); sulfolane (99%, *Merck*, Germany).

The selected compounds were used without prior preparation, with the exception of pentaerythritol (purified by repeated recrystallization to 99 wt % purity) and 2-ethylhexanoic acid (purified by fractional distillation to 99 wt % purity).

Experimental conditions

The esterification was carried out in a perfect-mixing apparatus, which consisted of a jacketed glass reactor (*RULLAB*, Russia) equipped with a sample collector and a Dean-Stark condenser. The temperature of the reaction zone (383.2, 393.2, and 403.2 K) was maintained using an oil bath (*Huber*, Germany) by circulating the heat transfer fluid polymethylsiloxane PMS-200 (*Acros Organics*, USA). The molar ratio of pentaerythritol to carboxylic acid was 1 : 8 in all cases. A combination of sulfolane (30 wt % of the reagent load) and methanesulfonic acid (1 wt % of the reaction mixture) was used as the catalytic composition.

Analysis of reaction systems

The reaction system was analyzed using gas-liquid chromatography on a Kristall 2000M instrument (*Khromatek*, Russia), which was equipped with a capillary column (60 m × 0.32 mm × 0.5 μm) with a grafted stationary phase BP-1 (100% dimethylpolysiloxane, *Khromatek*, Russia) and a flame ionization detector. Conditions: isothermal mode; column temperature 523.2 K (isobutanoates, *n*-pentanoates and their isomers, *n*-hexanoates and their isomers), 543.2 K (*n*-heptanoates), 593.2 K (*n*-octanoates, 2-ethylhexanoates, nonanoates), 593.2 K (decanoates); evaporator temperature 623.2 K; detector temperature 623.2 K; gas split ratio 1 : 50; carrier gas—helium; sample volume—0.15 μL. The concentration of pentaerythritol esters was determined using the internal standard method (calibrated against previously obtained pentaerythritol tetraesters and purified pentaerythritol over a wide concentration range).

The amount of reacted carboxylic acid was determined by acid–base titration. The balance amount of reaction water was calculated based on the concentrations of the

formed pentaerythritol esters in accordance with the stoichiometry of the reaction.

Determination of kinetic characteristics

The esterification of pentaerythritol with carboxylic acids comprises a reversible series of reactions consisting of eight forward and reverse reactions, which is described by the following reaction scheme.

Previous studies of a model reaction, as well as data from the literature [15, 16], indicate that the reactions in such systems have a total reaction order of two.

The following system of differential kinetic Eqs. (1)–(7) was used to describe the reaction rate in stages [17]:

$$\frac{\partial C_{PE}}{\partial \tau} = -k_1 C_{PE} C_{CA} + k_5 C_M C_W, \quad (1)$$

$$\frac{\partial C_{CA}}{\partial \tau} = -k_1 C_{PE} C_{CA} - k_2 C_M C_{CA} - k_3 C_T C_{CA} - k_4 C_T C_{CA} + k_5 C_M C_W + k_6 C_D C_W + k_7 C_T C_W + k_8 C_{TE} C_W, \quad (2)$$

$$\frac{\partial C_M}{\partial \tau} = k_1 C_{PE} C_{CA} - k_2 C_M C_{CA} - k_5 C_M C_W + k_6 C_D C_W, \quad (3)$$

$$\frac{\partial C_D}{\partial \tau} = k_2 C_M C_{CA} - k_3 C_D C_{CA} - k_6 C_D C_W + k_7 C_T C_W, \quad (4)$$

$$\frac{\partial C_T}{\partial \tau} = k_3 C_D C_{CA} - k_4 C_T C_{CA} - k_7 C_T C_W + k_8 C_{TE} C_W, \quad (5)$$

$$\frac{\partial C_{TE}}{\partial \tau} = k_4 C_T C_{CA} - k_8 C_{TE} C_W, \quad (6)$$

$$\frac{\partial C_W}{\partial \tau} = k_1 C_{PE} C_{CA} + k_2 C_M C_{CA} + k_3 C_D C_{CA} + k_4 C_T C_{CA} - k_5 C_M C_W - k_6 C_D C_W - k_7 C_T C_W - k_8 C_{TE} C_W, \quad (7)$$

where C_i is concentration, mol/L; τ is time, min; k_i is rate constant of the *i*th second-order reaction, L/(mol·min); abbreviations: PE is pentaerythritol, CA is carboxylic acid, M is pentaerythritol monoester, D is pentaerythritol diester, T is pentaerythritol triester, TE is pentaerythritol tetraester, W is water.

The systems under study consist of a series of reversible reactions; in order to describe them, the calculation was divided into two stages. The first stage of the calculation was performed over a very narrow initial time interval during which the concentration of the reaction water was negligible. This stage was treated as a set of irreversible reactions; the rate constants of the forward reactions were estimated using the initial rate method (the rate constants were calculated using Euler's method [18]), according to the system of Eqs. (8)–(12):

$$S_1 = \sum \left(C_{M_{calc}} - C_{M_{exp}} \right)^2, \quad (8)$$

$$S_2 = \sum \left(C_{D_{calc}} - C_{D_{exp}} \right)^2, \quad (9)$$

$$S_3 = \sum \left(C_{T_{calc}} - C_{T_{exp}} \right)^2, \quad (10)$$

$$S_4 = \sum \left(C_{TE_{calc}} - C_{TE_{exp}} \right)^2, \quad (11)$$

$$\sum_1^4 S_i \rightarrow \min, \quad (12)$$

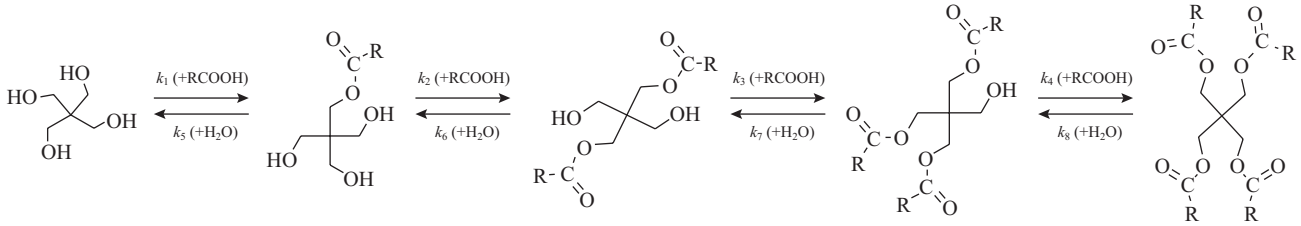
where S_i is the sum of the squares of the deviations between the calculated (calc) and experimental (exp) concentrations of the resulting esters.

The rate constants for the reverse reactions were calculated based on the equilibrium concentrations of the reactants and the obtained values of the forward reaction rate constants using Eq. (13):

$$\frac{k_{for}}{k_{rev}} = \frac{C_i C_j}{C_g C_l}, \quad (13)$$

where k_{for} and k_{rev} are the rate constants for the forward and reverse reactions, respectively, in L/(mol·min); C_i and C_j are the concentrations of the forward reaction products; C_g and C_l are concentrations of the reverse reaction.

The adequacy of the kinetic model was assessed using Pearson's criterion [19], which yielded a value of at least 96% for the entire series of experiments conducted.



Scheme. Transformations occurring during the interaction of pentaerythritol with carboxylic acids

RESULTS AND DISCUSSION

Equilibrium composition of reaction systems

Within the temperature range studied (383.2–403.2 K), chemical equilibrium was observed. The figure illustrates an example of the esterification of isopentanoic acid. The state of chemical equilibrium was confirmed by a fivefold increase in contact time from the moment equilibrium was established, which remained constant.

The composition of the equilibrium mixture (mono-, di-, tri-, and tetrapenterythritol esters) is shown in Table 1.

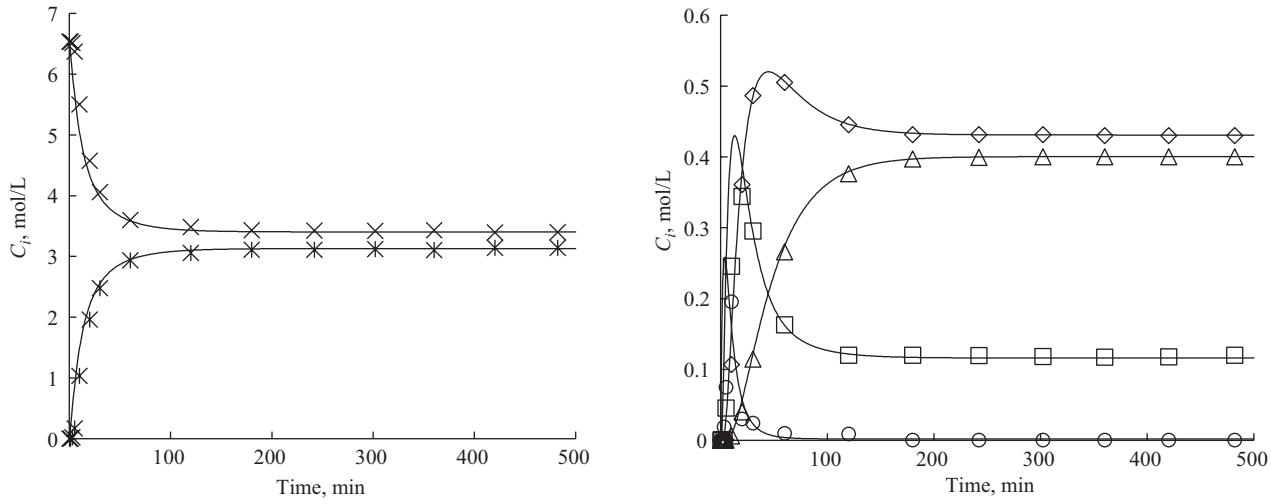


Fig. Concentration dependencies of the esterification of isopentanoic acid with pentaerythritol at a temperature of 383.2 K: (a) × — isopentanoic acid, ∗ — reaction water; (b) ○ — pentaerythritol monoester, □ — pentaerythritol diester, ◊ — pentaerythritol triester, Δ — pentaerythritol tetraester

Table 1. Equilibrium composition during esterification of carboxylic acids with pentaerythritol at 383.2 K

Pentaerythritol ester	Content of pentaerythritol esters in the equilibrium mixture, mol %			
	Monoester	Diester	Triester	Tetraester
Linear C_5–C_{10}	0.2 ± 0.1	3.8 ± 2.1	46.1 ± 3.7	49.9 ± 2.4
Pentaerythritol esters of isomeric acids C_4–C_8				
2-Methylpropanoate	0.6 ± 0.3	13.1 ± 1.9	47.9 ± 2.3	38.5 ± 5.3
3-Methylbutanoate	0.6 ± 0.4	12.2 ±2.7	45.6 ± 3.8	41.2 ±3.1
2,2-Dimethylpropanoate	0.4± 0.0	9.9± 2.4	44.5± 2.2	45.2± 4.1
2-Ethylbutanoate	0.5 ± 0.1	13.3 ± 3.7	44.5 ± 3.1	41.2 ± 2.0
2,2-Dimethylbutanoate	0.3 ± 0.2	10.2 ± 1.8	44.8 ± 2.9	44.7± 3.0
4-Methylpentanoate	0.9 ± 0.2	12.9 ± 2.0	39.5 ± 4.1	46.6 ± 2,7
2-Methylpentanoate	0.6 ± 0.1	12.1 ± 1.1	44.8 ± 4.1	42.6 ± 2.4
2-Ethylhexanoate	0.9 ± 0.3	12.7 ± 2.9	44.6 ± 2.9	41.9 ± 3.2

Analysis of the reported values shows that, under the synthesis conditions considered, the diester content is lower in compounds with a linear structure compared to those with an isostructural configuration. Otherwise, the compositions of the reaction mixtures are approximately the same, indicating similar equilibrium constants (which are practically independent of the structure of the carboxylic acid). It should be noted that pentaerythritol was absent in all reaction systems, indicating its 100% conversion.

Kinetic characteristics of esterification with pentaerythritol

From the experimental data in the temperature range 383.2–403.2 K, the rate constants for all studied systems were calculated using Eqs. (1)–(7), and the parameters of the Arrhenius equation (activation energy and pre-exponential factor) were estimated; these are presented in Table 2.

Table 2. Kinetic parameters of esterification of carboxylic acids with pentaerythritol

Direct reactions								
N	E_{a1}	$\lg(k_0)_1$	E_{a2}	$\lg(k_0)_2$	E_{a3}	$\lg(k_0)_3$	E_{a4}	$\lg(k_0)_4$
1–6	27.7	2.9	30.1	2.9	34.0	3.1	49.3	4.3
7	33.2	3.3	38.2	3.7	43.0	4.0	55.3	5.0
8	28.7	2.7	32.1	3.1	37.7	3.3	53.3	4.8
9	36.0	3.2	52.1	5.2	59.7	5.5	74.8	6.7
10	33.4	3.4	40.2	3.9	45.7	4.2	61.4	5.4
11	30.5	2.8	34.7	3.2	40.4	3.5	52.1	4.6
12	36.3	3.3	51.0	5.3	58.6	5.3	76.7	6.6
13	33.4	3.5	40.2	4.1	49.4	4.4	64.4	5.7
14	38.4	3.7	44.2	4.3	49.4	4.6	64.4	5.8
Reverse chemical reactions								
N	E_{a5}	$\lg(k_0)_5$	E_{a6}	$\lg(k_0)_6$	E_{a7}	$\lg(k_0)_7$	E_{a8}	$\lg(k_0)_8$
1–6			31.0	1.7	37.6	2.5	51.0	4.5
7			36.1	2.1	43.1	3.5	53.5	4.9
8			31.3	1.7	37.6	2.8	53.5	4.9
9			49.4	3.5	60.4	4.9	70.2	5.9
10		–	36.3	2.1	43.0	3.3	57.3	4.9
11			31.3	1.6	38.6	2.8	52.4	4.6
12			49.7	3.4	62.2	4.8	72.3	6.0
13			36.3	2.2	43.4	3.1	57.3	4.8
14			36.3	2.1	42.1	3.1	57.3	4.9

Note: N is the number assigned to the carboxylic acid, given in the Materials and Methods section; the indices assigned to the parameters of the Arrhenius equation correspond to the numbers of the reaction stages (see the transformation diagram); E_{ai} is the activation energy of the ith reaction, kJ/mol; $\lg(k_0)_I$ is the decimal logarithm of the pre-exponential factor of the Arrhenius equation, which has the dimension under the logarithm sign L/(mol·min); the confidence interval of the values of the parameters of the Arrhenius equation is at the level of ±5%.

Analysis of the data in Table 2 confirms that the reaction rate depends significantly on the structure of the carboxylic acid. This is reflected in the values of the pre-exponential factor of the Arrhenius equation and the activation energy. The lowest value was obtained for linear carboxylic acids and increases with increasing degree of branching.

The esterification of pentaerythritol with linear carboxylic acids to mono-, di-, and triesters proceeds in virtually the same manner, as evidenced by similar values for the activation energy (27.7–34.0 kJ/mol) and the pre-exponential factor (2.9–3.1 L/(mol·min)) in the order of magnitude of the decimal logarithm. Upon further esterification to a tetraester, an increase in the values of both parameters is observed (49.3 kJ/mol and 4.3 L/(mol·min), respectively). This is due to the presence of a significant steric hindrance that impedes the reaction proceeding via the terminal hydroxyl group. In the presence of branching in the carboxylic acid molecule, this effect manifests itself already in the early stages of esterification, becoming stronger with an increase in the number of substituents and their size (especially when they are present at the α-carbon atom). This may explain the difference in the amount of diesters between linear and branched carboxylic acids used in the experiment.

Taken together, the data obtained can be regarded as the necessary foundation for developing technological processes aimed at controlling the chemical reaction through thermodynamic (equilibrium) and kinetic control. Thermodynamic control is feasible when producing technical mixtures consisting primarily of a mixture of tri- and tetraesters with only trace amounts of diesters. Moreover, this approach is identical for all reaction substrates: the independent composition of the structure of the carboxylic acid is confirmed by experimental data. However, the selective production of a particular ester is possible only through kinetic control by varying various process conditions: the reagent ratio, reaction temperature, and contact time.

In practice, synthetic oils based on pentaerythritol esters are produced by esterifying pentaerythritol with a fraction of synthetic C_5–C_{10} fatty acids. Unfortunately, these fractions are characterized by an inconsistent component composition, which inevitably leads to changes in the properties of the commercial oil. Thus, knowledge of the kinetic characteristics is necessary for successful process modeling when using mixed feedstocks in order to be able to predict the behavior of the reaction substrate by optimizing process parameters.

CONCLUSIONS

For the first time, the catalytic esterification of 14 carboxylic acids of various structures with pentaerythritol in a sulfolane medium has been carried out. The equilibrium compositions of the esterification products have been determined experimentally. The equilibrium composition of the reaction products is shown to be practically independent of the structure of the carboxylic acid. After determining the rate constants for the systems under consideration, the parameters of the Arrhenius equation were estimated for the forward and reverse reactions. The main constraints on the kinetic component of the process are shown to be imposed by steric hindrances due to the structure of the carboxylic acid. The obtained data will support validated kinetic models that enable the design of syntheses for target esters with high selectivity and predictable properties through thermodynamic or kinetic control of the esterification process.

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Authors' contributions

Yu.F. Ivanova— conducting the experiment, discussion of experimental data, writing the text of the article.

V.V. Emelyanov—experimental data processing, discussion of experimental data, writing the text of the article.

S.V. Levanova—discussion of experimental data, writing the text of the article.

The authors declare no conflicts of interest.

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