

Techno-Economic Analysis of an Improved Process for Producing Saturated Branched-Chain Fatty Acids

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Abstract

Methyl-branched fatty acids produced by isomerization of oleic acid ('isostearic' acids (IA)) are industrially useful products with excellent thermostabilities and lubricities and reduced freezing points relative to stearic acid. They have potential utility as biodiesel or a biodiesel additive imparting improved low temperature fluidity. We present a techno-economic model for industrial scale production of isostearic acid by zeolite-catalyzed isomerization. A catalyst regeneration loop allowing 20 reaction cycles was included. Use of catalyst for 15 or more reaction cycles reduced process cost by 51% vs. a single use reaction format. However, with a best-case predicted production cost of \$2.375/kg (\$1.080/lb), further process cost reductions will be required before use of IA esters as high percentage blend components of biodiesel is economically feasible.

Keywords: branched-chain fatty acids, ferrierite, isostearic acid, SuperPro Designer, techno-economic, zeolite

1. Introduction

The 2002 United States Farm Bill encouraged the use of biobased products; however, they must be economical, functional, and readily available (Schnepf, 2013). Biobased products can be derived from carbohydrates, proteins and lipids. Thus, they are generally more environmentally friendly materials and have lower toxicity when compared to petroleum-based materials. Fatty acid derivatives from fats and oils are being used in the biodiesel, lubricant, personal care, polymer, and surfactant industries. Although biobased products have many advantages over petroleum-based products, the high costs of some of the finished products have limited their adoption. To overcome this obstacle, research efforts to develop economically feasible technologies for the production of biobased materials are necessary, and these technologies and the products they generate must be competitive with or superior to petroleum-based processes and products.

Branched-chain fatty acids such as commercial isostearic acid (IA) are unique chemicals because of their novel and interesting properties (Ngo, Dunn, Sharma, & Foglia, 2011). They are found in minor amounts in nature and are produced by industry in bulk quantities (Anderson & Chargaff, 1929; Hayes, 1988). IA is a family of 17-carbon straight chain fatty acids containing a methyl group at any of various positions of the alkyl chain backbone (Figure 1) (Polgar, 1970). Steric consequences of the methyl branch cause reductions in the melting point of the fatty acid, yielding a potential biodiesel feedstock or lubricant with improved low temperature performance relative to the unbranched parent compound. Thus IA and their derivatives are used in applications such as body washes, coatings, cosmetics, lubricant additives, hydraulic fluids, and emulsifiers (Townend et al., 2012; Benoit, 1963; Sayad, 1967; Landfried & Bassett, 1970). They have potential utility as low temperature compatible biodiesels or biodiesel additives. CRODA Co. currently manufactures IA under the trade name PrisorineTM (P3505 ISAC) and Arizona Chemical, another leading oleochemical company, produces IA under the trade names CenturyTM 1105 and 1107.



Figure 1. Isostearic acid

Dashed lines indicate several possible positions for the branching methyl group.

The existing technology for IA production involves clay-catalyzed oligomerization of tall oil fatty acid (Hayes, 1988). This process involves reactions with small amounts of water performed in stainless steel reactors at high temperature (180-260 °C) and pressure (up to 10 bars). Generally, this reaction results in the formation of a mixture of monomeric (10-40% saturated and unsaturated branched-chain fatty acids) and predominantly oligomeric (60-80% C₃₆-dimer fatty acids) species (Hayes, 1988). Dimer fatty acids have two carboxylic groups and an alkyl chain in an open or cyclic form. The exact compositions of dimer fatty acids depend on the catalysts and feedstocks used for their production. The chemical structures, physical properties and yields for these two fractions are quite different, and as a result, they are typically sold in two different markets (Anonymous, 2006). IA are made in limited production capacity and sold in the relatively higher value markets mentioned above. The dimer products enter the polyamide sector, and are considered to be in oversupply. Their prices can be half that of IA.

The currently employed clay catalyst technology for IA production has two major drawbacks. First, the reaction gives predominantly oligomeric by-products (mainly dimers and trimers) and thus exhibits a rather low yield of IA. Second, there is no data to indicate that clay catalysts can be reused, leading to a costly process with a negative environmental impact due to the burden of disposing the catalysts. Thus, there exists a need for more efficient and renewable processes for the production of IA.

In order to improve on the existing clay-catalyzed technology, several parameters could be considered. First, the initial catalyst cost could be lowered; second, the catalyst efficiency could be improved; third, the catalyst could have good recycling ability with acceptable levels of retained activity after regeneration; fourth, the catalyst could be an easily recovered one; and finally, the value of the synthesized product could be improved over that currently produced. We have sought to develop technologies to meet these criteria.

We (Ngo et al., 2007, 2011, 2012) and others (Hodgson, 1996; Tomifuji et al., 1997; Zhang et al., 2003, 2004, 2005) have previously described a zeolite catalyzed isomerization process for producing IA which appears to be promising alternative approach to the current clay technology. To evaluate the economic feasibility of this new process, computer modeling software such as Superpro Designer (Intelligen Inc., Scotch Plains, NJ) and Aspen Plus (Aspen Technology Inc., Burlington, MA) are commonly used to predict the capital and operational costs of a technology. Superpro Designer is a highly valuable tool by which scientists and engineers can assess the economics, process development needs, and environmental impacts of a technology before committing to a full scale implementation and commercialization. These tools have been successfully applied to determine the economic costs and feasibilities in various technology areas, including biodiesel production from refined soybean (Haas et al., 2006), rapeseed (Abo El-Enin et al., 2013), and algal oils (Taylor, et al., 2013). We have previously used this software to model H-Ferrierite zeolite catalyzed branching of oleic acid to produce IA (Ngo et al., , 2012). This model (Model 1) employed a catalyst regeneration technology that allowed catalyst to be reused for a total of at least 5 reaction cycles (Ngo et al., 2012). It predicted that the process could have significant positive impact on the economics of branched-chain fatty acid production, and the fact that the catalyst was recyclable greatly influenced the economics of the overall process (Ngo et al., 2012). Encouraged by this work, we have further refined the process, identifying an improved zeolite regeneration protocol that allows further reuse of the catalyst, potentially decreasing capital costs and energy consumption. In this paper, modified catalyst regeneration protocols that add either acid or heat treatment steps to the process are presented. Four techno-economic models for the production of branched-chain fatty acid products from oleic acid are presented and discussed.

2. Results and Discussion

2.1 Description of the Process Model

The economic impact of saturated branched-chain fatty acid isomer production using various catalyst

regeneration protocols was evaluated by the computer simulation software SuperPro Designer (version 8.5. build 6). Similar to the previously reported model (*i.e.*, Model 1) (Ngo et al., 2012), this new model (*i.e.*, Model 2) was designed to operate for 330 days per year, 24 h per day with a plant capacity of 4.5 million kg yr⁻¹ (10 million lb yr⁻¹). Model 2 differed from Model 1 in that Model 2 is based on a protocol involving 20 cycles of use whereas the previous model included only 5 catalytic cycles of use. The flow diagram for Model 2 is shown in Figure 2 and detail descriptions of Figure 2 can be found in the previously reported publication (Ngo et al., 2012). All processes modeled here were assumed to operate continuously. Continuous reactors have advantages over batch reactors in terms of their greater amenability to automatic control and operation. They have better quality control of the product lines over the batch process, and they reduce labor costs and stabilize operating conditions.

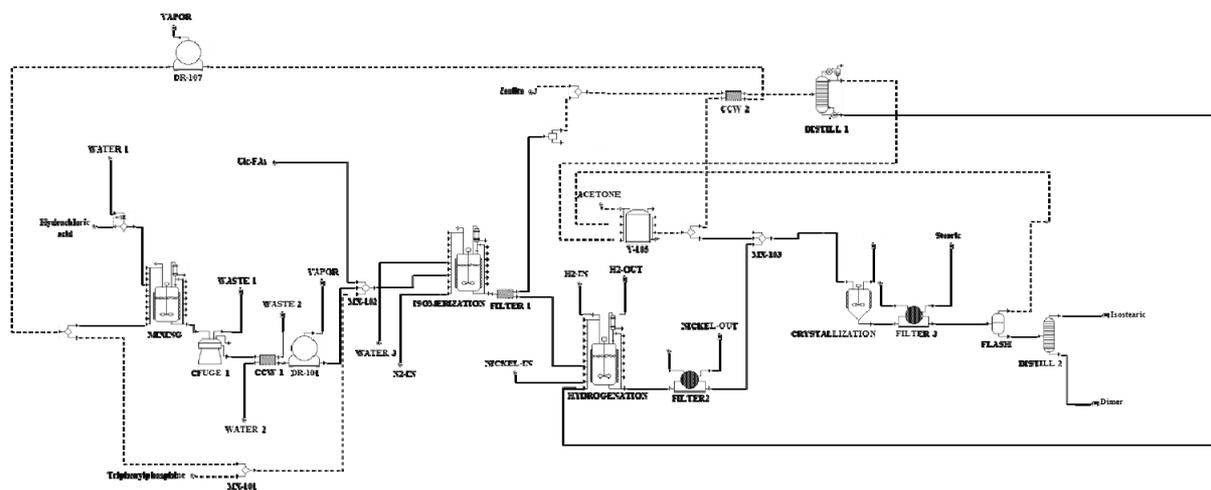


Figure 2. Flow diagram of isostearic acid technology

As in the previous model (Model 1) (Ngo et al., 2012), Model 2 was divided into three processing sections, namely (1) catalyst treatment and regeneration, (2) isomerization, and (3) product recovery. Dashed lines in Figure 2 identify new streams in the process relative to Model 1. By using an improved catalyst regeneration protocol, developed in our laboratory, we have shown that it is possible to use the catalyst at least 20 times without significant loss of catalytic activity. The ability of this catalyst regeneration protocol to allow retention of substantial catalyst activity and selectivity in multiple successive reactions is shown in Table 1. Detailed procedures for obtaining the experimental data were reported previously (Ngo, 2014). In Model 1, the branched-chain fatty acid product was produced by isomerization of oleic acid in the presence of catalytic amounts of H-Ferrierite zeolite and distilled water at 260 °C for 4 h. After isomerization, the spent H-Ferrierite zeolite catalyst was recovered, washed with acetone to remove adsorbed lipid, dried, and regenerated by washing with dilute hydrochloric acid (Ngo, 2014). In Model 2, the catalyst was also recovered after isomerization, and acetone washed (Figure 2, CCW 2). Rather than proceeding to an acid wash step for regeneration, however, Model 2 implements a heat treatment step at this point (115 °C, 20 h, Figure 2, DR-107) since we recently determined that this treatment can routinely substitute for most acid washing steps. By the 5th regeneration cycle, however, the catalyst shows a slight drop in activity (Table 1). We have found that an acid regeneration step at this point alleviates this activity loss, and thus an acid wash occurs in Model 2 after each five reaction cycles.

Table 1. Ability of regeneration to restore/retain zeolite catalytic activity and selectivity in consecutive isomerizations of oleic acid to isostearic acid^a

Entry	Run	TPP [wt%]	GC wt%	% conversions ^b
			Isostearic acid	
1 ^c	1	7.5	82	99
2	2	0	81	98
3	3	0	80	98
4	4	0	77	97
5	5	0	75	93
6 ^c	6	2.5	84	99
7	7	0	77	95
8	8	0	78	97
9	9	0	77	96
10	10	0	75	93
11	11	0	73	92
12 ^c	12	2.5	82	98
13	13	0	81	98
14	14	0	77	95
15	15	0	70	89
16	16	0	78	96
17	17	0	75	95
18 ^c	18	2.5	80	98
19	19	0	80	94
20	20	0	80	94

^aGC data collected on the intact reaction product after isomerization, hydrogenation and methylation using methyl tridecanoate as internal standard. Reactions were carried with 5 wt% H-Ferrierite, TPP, 1.8mL distilled water at 260 °C for 4 h.

^bConversion calculated as $94.3 - [(methyl\ stearate - 5.74)]/94.3 \times 100$ [94.3 is the total unsaturated fatty acids in the starting fatty acids (oleic acid). 5.74 is the fatty acids in the oleic acid which do not contribute to the reaction].

^cFresh and spent zeolite catalysts were treated with dilute HCl acid solution in the presence of TPP.

Note: TPP=Triphenylphosphine.

In addition, in Model 2 as opposed to the previous model, each acid wash is followed by the addition of triphenylphosphine (TPP) to the subsequent isomerization reaction. The TPP treatment was added since we have recently learned that the addition of a small amount of TPP (2.5 to 7.5 wt% to zeolite catalyst) to the isomerization reaction suppresses the formation of dimer fatty acid product (Ngo, 2014), thus boosting isostearic acid yields (Table 2). The acid wash strips some TPP from the catalyst (data not shown), necessitating this TPP addition after each wash (Figure 2, MX-101). The heat and acid-TPP treatments can be repeated in multiple cycles (Table 1), a feature embodied in Model 2 to achieve a total of 20 uses of catalyst.

Table 2. Product yields derived from the process model

	Model 1 ^a		Model 2 ^b	
	Flow Rate (kg yr ⁻¹)	Yield (%)	Flow Rate (kg yr ⁻¹)	Yield (%)
<u>Input</u>				
oleic acid (91.2 wt% C18:1)	5,628,796	---	5,628,796	---
<u>Output</u>				
isostearic acid	4,529,317	78.6	5,089,626	86.2
stearic acid	476,253	8.30	574,429	9.73
dimer FAs	752,069	13.1	238,103	4.07
<u>Total</u>	5,757,639	100	5,902,158	100

^aModel 1 is a model previously reported in Ngo et al. (2012).

^bModel 2 is the new improved model reported here.

The acetone recovered from the catalyst wash step was purified by distillation (Figure 2, DISTILL1). Acetone from the distillation column and the flash tank, (Figure 2, FLASH) was collected in Tank V-105 (Figure 2) and redistributed for use in the catalyst washing and product recrystallization steps. Since the initial products are unsaturated and the item of commerce is saturated, hydrogenation of the initial product is necessary (Figure 2, HYDROGENATION). A small amount of residual fatty acids from the distillation column was recycled back to the hydrogenation reactor. Detailed descriptions of the hydrogenation reaction and the product isolation operations can be found in Model 1 (Ngo et al., 2012).

2.2 Plant Operation and Analysis

As indicated in Table 2, Model 2, for this industrial scale model the oleic acid input was 5,628,796 kg (12,405,866 lb) and the outputs for the three products were 5,089,626 kg (11,217,535, lb) of IA, 574,429 kg (1,266,041 lb) of saturated linear-chain fatty acid, and 238,103 kg (524,779 lb) of dimer fatty acids. To evaluate the productivity gain of Model 2, the productivity was expressed in terms of the total amount of product (kg) obtained per kg catalyst employed for Models 1 and 2. The results showed a productivity gain of 105% from Model 1 (204.6 kg/kg) to Model 2 (419.5 kg/kg). This improved process of Model 2 generates a much larger amount of branched-chain fatty acid product and a substantially smaller amount of dimer product than achieved with Model 1 due to the use of TPP after each acid wash, as described above.

Table 3 lists the capital costs of Models 1 and 2. Capital costs were based on an engineering factored estimate developed from the costs of the individual equipment items necessary for the process. An additional allowance of 15% was added to these equipment costs to cover the processing equipment items that could not be defined at this time but would be required for the process. The total capital cost was then generated from these equipment prices by using a capital cost to equipment ratio of 3 to cover all other costs of construction materials and installation, engineering, and other charges associated with the construction of an industrial facility (Table 3). There was a slight increase in capital cost for the improved process of Model 2 because of the additional equipment needed for the zeolite treatment and regeneration. The costs of the other steps (*i.e.*, isomerization, hydrogenation, product recovery) also went up slightly because of the larger tanks needed for this facility when compared to the Model 1 facility. Overall, the capital cost of the Model 2 process is approximately 3% greater than that of Model 1, which is minimal given that this is calculated on a 10 year depreciation basis.

Table 3. Predicted isomerization facility capital costs of the improved model

	Model 1 ^a		Model 2 ^b	
	Equipment cost (\$)	Capital Cost (\$) ^c	Equipment cost (\$)	Capital Cost (\$) ^c
<u>1. Catalyst Treatment & Regeneration</u>				
Hydrochloric acid handling & storage	34,000		34,000	
Make up zeolite handling & storage	35,000		35,000	
Zeolite activation	68,000		36,000	
Zeolite filtering & centrifugation	124,000		124,000	
Zeolite drying	46,000		92,000	
Unlisted equipment for the zeolite area	53,000		56,000	
Catalyst treatment area total	360,000	1,080,000	377,000	1,131,000
<u>2. Isomerization & Hydrogenation</u>				
Oleic acid storage & handling	65,000		66,000	
Isomerization reactor	429,000		437,000	
Zeolite separation	48,000		48,000	
Nickel catalyst storage & handling	35,000		35,000	
Hydrogenation reactor	50,000		50,000	
Catalyst & vapor removal	59,000		60,000	
Unlisted equipment for isomerization area	119,000		121,000	
Isomerization & Hydrogenation area total	805,000	2,416,000	817,000	2,451,000
<u>3. Product recovery</u>				
Acetone storage & handling	34,000		34,000	
Recrystallization reactor	394,000		400,000	
Stearic separation & storage	147,000		119,000	
Acetone recovery	272,000		333,000	
Isostearic/dimer distillation column	53,000		56,000	
Isostearic storage & handling	34,000		34,000	
Dimer storage & handling	34,000		34,000	
Unlisted equipment for product recovery area	168,000		175,000	
Product recovery area total	1,136,000	3,409,000	1,185,000	3,555,000
Total system cost	2,301,000	6,905,000	2,379,000	7,137,000

^aModel 1 is a model previously reported in Ngo et al. (2012).

^bModel 2 is the new improved model incorporating 20 reuses of the catalyst.

^cCapital cost is generated from the equipment prices by using a capital cost to equipment ratio of 3 to cover all other costs of construction materials and installation, engineering, and other charges associated with the construction of an industrial facility.

Table 4 lists the annual operating costs, which includes material, utility, labor, and facility expenses for the two models. As shown, there is a significant saving with the new model because of the decrease in catalyst cost from Model 1 to 2 due to catalyst regeneration (*i.e.*, 10.6 % to 5.5%). However, there are minor aspects which cause the unit production cost to go up, such as excess acetone and TPP employed in catalyst regeneration. Overall,

Model 2 has a predicted unit product cost that is $\$0.16 \text{ kg}^{-1}$ ($\$0.07 \text{ lb}^{-1}$) less than for Model 1. This is equivalent to a substantial savings of about \$575,000 annually. These results clearly show the importance of catalyst efficiency and recyclability.

Table 4. Predicted annual operating costs of Models 1 and 2

Annual operating cost summary	Model 1 ^a		Model 2 ^b		Difference between two models
	Annual cost (\$)	Annual cost (%)	Annual cost (\$)	Annual cost (%)	Annual cost (\$)
<u>Material Costs</u>					
oleic acid (91.2 wt%)	9,344,000	64.0	9,344,000	66.7	0
zeolite ferrierite	1,548,000	10.6	774,000	5.5	774,000
nickel on silica	862,000	5.9	862,000	6.2	0
acetone	400,000	2.7	496,000	3.5	(96,000)
triphenylphosphine	0	0	19,000	0.1	(19,000)
other raw materials	164,000	1.1	174,000	1.2	(10,000)
<u>Utilities</u>					
electricity	123,000	0.8	137,000	1.0	(14,000)
steam	261,000	1.8	280,000	2.0	(19,000)
cooling agents	92,000	0.6	102,000	0.7	(10,000)
<u>Labor</u>					
2 operators / shift	792,000	5.4	792,000	5.7	0
<u>Facility Expenses</u>					
		0			0
depreciation	691,000	4.7	712,000	5.1	(21,000)
other facility expenses	314,000	2.2	324,000	2.3	(10,000)
<u>Total</u>	14,591,000	100	14,016,000	100	575,000

^aModel 1 is a model previously reported in Ngo et al. (2012).

^bModel 2 is the new improved model incorporating 20 reuses of the catalyst.

To explore the possibility of further reducing the cost of zeolite-catalyzed IA production, three additional process models (*i.e.*, Models 3, 4 & 5, Table 5) were developed, based on Model 2. These differ from the parent model in lacking certain process steps, in an attempt to evaluate the potential savings to be gained from their elimination.

Model 3 is similar to Model 2 except that a dryer (Figure 2, DR-107) has been removed from the process just downstream of the acetone washing of the catalyst during regeneration. It served to dry the catalyst with a treatment of 115 °C for 20 h. The unit production cost for IA synthesis by the process of Model 3 was $\$0.008 \text{ kg}^{-1}$ ($\$0.004 \text{ lb}^{-1}$) less than that for Model 2. Thus, there is little financial motivation to explore eliminating the catalyst drying step from the process.

Table 5. Predicted annual operating costs of various catalyst treatment method studies

Annual operating cost summary	Model 2 ^a		Model 3 ^b		Model 4 ^c		Model 5 ^d	
	Annual cost (\$)	Annual cost (%)						
Material Costs								
oleic acid (91.2 wt%)	9,344,000	66.7	9,344,000	66.9	9,344,000	65.6	9,344,000	66.6
zeolite ferrierite	774,000	5.5	774,000	5.5	774,000	5.4	774,000	5.5
nickel on silica	862,000	6.2	862,000	6.2	862,000	6.1	862,000	6.1
acetone	496,000	3.5	474,000	3.4	507,000	3.6	498,000	3.6
triphenylphosphine	19,000	0.1	19,000	0.1	187,000	1.3	19,000	0.1
other raw materials	174,000	1.2	175,000	1.3	178,000	1.3	174,000	1.2
Utilities						0.0		
electricity	137,000	1.0	137,000	1.0	141,000	1.0	138,000	1.0
steam	280,000	2.0	278,000	2.0	284,000	2.0	281,000	2.0
cooling agents	102,000	0.7	102,000	0.7	101,000	0.7	103,000	0.7
Labor								0.0
2 operators / shift	792,000	5.7	792,000	5.7	792,000	5.6	792,000	5.6
Facility Expenses								
depreciation	712,000	5.1	697,000	5.0	735,000	5.2	712,000	5.1
other facility expenses	324,000	2.3	317,000	2.3	335,000	2.4	324,000	2.3
Total	14,016,000	100	13,971,000	100	14,240,000	100	14,021,000	100

^aModel 2 is the new improved process, involving 20 catalyst reuses with regeneration by heat treatment (115 °C, 20 h) after each use and dilute HCl/TPP treatment (55 °C, 24 h) after every 5th use.

^bModel 3 is a variant of Model 2 implementing 20 catalyst use cycles without drying after solvent washing.

^cModel 4 is a variant of Model 2 implementing 20 catalyst use cycles, with acid treatment and 5 wt% TPP added followed by heat treatment at 115 °C for 20 h after each use.

^dModel 5 is a variant of Model 2 implementing 20 catalyst use cycles with heat treatment at 260 °C for 4 h instead of 115 °C for 20 h after each.

In Model 4 the catalyst was regenerated with acid and 5 wt% TPP after each use rather than heat. Due to additional reagent costs of TPP, the unit production cost for this model was \$2.416 kg⁻¹ (\$1.096 lb⁻¹), an increase of \$0.041 kg⁻¹ (\$0.019 lb⁻¹) compared to Model 2. This is attributable to the resulting net higher consumption of TPP used in the process, as shown in Table 5. This emphasizes the greater economy of using heat regeneration (Model 2) rather than acid-TPP (Model 4) when possible.

In Model 5 the effect of using an alternate heat treatment of the catalyst, with heating at 260 °C for 4 hours instead of 115 °C for 20 hours after each use, was explored. The higher temperature/shorter time regime was chosen because it is known that catalyst regeneration occurs at that temperature (data not shown) and it was postulated that the shorter time of treatment might reduce energy costs. However, the unit production cost for this model was \$2.376 kg⁻¹ (\$1.078 lb⁻¹), compared with \$2.375 kg⁻¹ (\$1.077 lb⁻¹) for Model 2, an insignificant difference.

Using the techno-economic model a sensitivity study was conducted to evaluate the effect on IA production cost of implementing various degrees of catalyst reuse within the process. For a single-use process the model predicted an estimated unit production cost of \$4.917 kg⁻¹ (\$2.231 lb⁻¹). As the extent of catalyst reuse increased the unit production cost decreased (Figure 3). The degree of this reduction was most pronounced over the course of the first five uses, being cut nearly in half in the 5-use model (*i.e.*, \$2.769 kg⁻¹ (1.256 lb⁻¹)). With continued catalyst reuse the rate of cost reduction decreased substantially and the process cost essentially leveled off at \$2.419 kg⁻¹ (\$1.097 lb⁻¹) at 15 uses. This indicates the point where the reduction in the cost of catalyst as a

consequence of regeneration and reuse becomes insignificant compared to the total operating cost of the process.

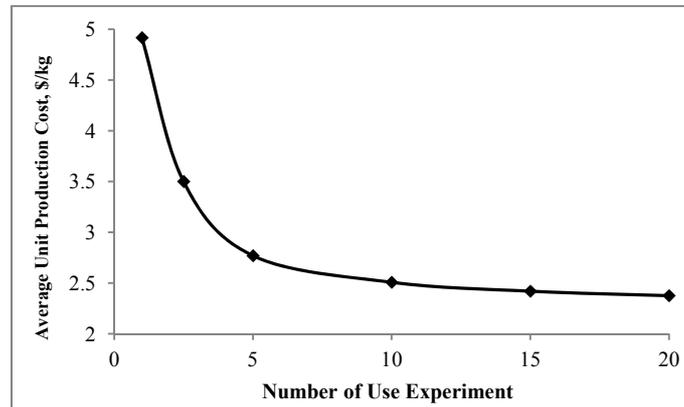


Figure 3. Impact of isomerization catalyst reuse on the unit production cost

3. Conclusions

There is a significant cost saving in the isostearic acid manufacturing process upon adopting the newly developed branched-chain zeolite technology. The high yields of the branched-chain product, the low formation of byproduct, and the facile catalyst regeneration protocols play significant roles in reducing the overall production costs. The process modeling studies here help identify the key areas that need to be improved and demonstrate the commercial viability of the technology. These modeling studies could help transition the developed branched-chain technology from research into industrial scale production and develop environmentally friendly and economically feasible engineering processes for other high-value biobased products. Thus, the skeletal isomerization approach for large scale production of biodegradable lubricants and hydraulic fluids could have both a positive environmental and industrial impact.

4. Future Perspective

Worsening global climatic conditions are likely to increase interest in the development of biobased replacements for today's petroleum-derived industrial products, be the fuels or nonfuels. In the context of biodiesel, poor low temperature fluidity is the single greatest property limiting its complete fungibility with the existing fuel pool. Thus, the development of biodiesel or biodiesel additives that improve the low temperature fluidity of biodiesel facilitate its adoption and will help ameliorate climate change. Similarly, development and adoption of other biobased industrial materials further fosters petroleum displacement. Isostearic acid can have uses in both fuel and nonfuel applications. Discovery of improved methods for their production will hasten their adoption. Development of techno-economic models to assess their production costs both allow quantitative assessment of these costs and help focus future research efforts to develop new technologies that reduce costs at the most expensive steps.

5. Executive Summary

- A techno-economic model constructed using laboratory-scale data for the industrial scale zeolite-catalyzed isomerization and subsequent hydrogenation of oleic acid to produce isostearic acid indicated a process cost of $\$4.917 \text{ kg}^{-1}$ ($\$2.231 \text{ lb}^{-1}$) when the catalyst was discarded after a single reaction cycle.
- By implementing a catalyst regeneration technology developed in this laboratory a profound reduction in process cost was achieved.
- The minimum predicted IA production cost was $\$2.375 \text{ kg}^{-1}$ ($\$1.080 \text{ lb}^{-1}$), attained upon use of the catalyst in 15 or more reaction cycles. This is a 51% reduction in cost relative to use of the catalyst in only one reaction.
- Substantial further cost reductions will be required to facilitate the use of e.g. methyl IA as a high percentage blend component to improve the low temperature fluidity of conventional biodiesel.

6. Key Terms

Isostearic acid: Traditional chemical name for the family of fatty acid positional isomers composed of a 17 carbon straight chain fatty acid backbone from which a single methyl group branch extends. Largely industrial

products derived by isomerization and reduction of oleic acid (C18:1). The methyl branch is located at different positions of the carbon chain in the various isomers of the family, which are not generally available as pure species. These low-melting species display desirable lubricities and oxidative stabilities and are used in applications requiring these properties. Wider adoption is pending development of reduced-cost production technologies.

Ferrierite zeolite: Ferrierite zeolite is commercially available and has been used in the skeletal isomerization of butene to iso-butene. However, Ferrierite has not been previously examined for skeletal isomerization of fatty acids. It has 2-dimensional open channels of $5.4 \times 4.2 \text{ \AA}$ formed by 10-membered rings (10-MR) that are interconnected by smaller channels of $4.8 \times 3.5 \text{ \AA}$ formed by 8-MR. The channels are ideal for enhancing the transport of oleic acid starting materials and isostearic acid products.

Techno-economic analysis/modeling: An approach to estimating the cost of a technological process, combining process modeling, engineering design and economic information to provide quantitative and qualitative assessments of capital and process costs. It is generally applied at industrial scales. In addition, its capability for sensitivity analysis allows this approach to identify process steps associated with highest costs, thereby allowing the efficient focus of research efforts on improving the economics of these steps.

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