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COMPUTER SIMULATION AND ANALYSES OF GLACIAL-GRADE ACRYLIC ACID PRODUCTION VIA THE CATALYTIC OXIDATION OF PROPYLENE

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ABSTRACT

A model and calculation technique that supports the design of acrylic acid (AA) production process using ChemCAD simulation software has been described. In order to produce AA a two-step process of vapor phase partial oxidation of propylene was selected. This optimization involved more investigation of recover acrylic from the gaseous reactor effluent rather than native reaction kinetic characteristics. A new simple procedure for further separation process of reactor products has been developed. The hot gaseous effluent reactor is cooled to 263 K in a condenser whereby its separates light non-condensable gases such as nitrogen, oxygen, carbon dioxide, etc. The resulting condensate is fed to a further separation process in two series-connected distillation columns. As a result, a liquid bottom stream of the final column containing AA with 99.9 mol% purity is obtained. The top stream of the same column is returned for recycling to the reactor section. Several sensitivity studies were carried out: influence of the condenser operating temperature (1) and pressure (2) in the obtained amounts of AA and acrolein; influence of the number of stages (3, 4), reflux ratio (5, 6) and number of feed stages (7, 8) for both distillation columns on the amount of AA produced therein. As a results an optimization of the condenser and distillation columns were carried out. A complete computer simulation at all parts of the flow sheet for the production of AA through partial oxidation of propylene has been made.

Keywords: computer simulation, catalytic oxidation, acrylic acid, sensitive analyses, ChemCAD.

INTRODUCTION

Acrylic acid (AA) is a commonly used as a precursor for a production of polymers [1, 2], textiles, and numerous other industrial and consumer products. AA is applied to make acrylates [3] and esters (accounting for 55 % of global demand) [4]. Polyfunctional allyl ethers of sucrose have been copolymerized in minor proportions with acrylic acid to give branched water-soluble copolymers useful as synthetic mucilages [5]. AA can form interpenetrating polymer network (IPN) hydrogels with other natural or synthetic polymers [6]. Because of the lucrative market for AA, this investigation focuses on the optimization of an acrylic acid manufacturing process. Two grades of AA are commercially available: technical-grade and glacial-grade. Technical, or crude AA is approximately 94 % purity by mass. Glacial (industrial) or polymer AA is generally 99.5 % to 99.7 % AA by mass and is polymerized to produce polyacrylic acid-based polymers.

There are several chemical pathways to produce AA, but the most common one is via the partial oxidation of propylene. To determine the effective heat transfers as well as kinetic parameters of propylene oxidation process different kinetic reaction scheme has been investigated [7, 8]. One alternative is the direct catalytic oxidation of propylene to AA in a single phase and single reactor. Several studies on the reaction pathway for the direct oxidation of propylene to AA activated by mixed oxides have been published [9 - 13]. The process requires maintaining the temperature between 325 °C and 350 °C in order to attain an economically reasonable propylene conversion, but under these conditions, significant total oxidation occurs, which causes a decrease of selectivity. Moreover, the catalyst shows significant deactivation.

Another alternative involves the conversion of propylene to acrolein, and then conversion of acrolein to AA in the second catalytic oxidation step [7]. In this case a higher selectivity is possible by optimizing the catalyst composition and reaction conditions for each of the steps in the two-stages oxidation process. Highly active and selective catalysts maximize both the yields of propylene to acrolein in the first step and then the conversion of acrolein to AA in the second step [14 - 16]. As a result a more efficient utilization of raw material has been found. Due to this reason the two stages oxidation process finds favor over the single-stages process in most commercial facaties and it has been used in this study.

When AA is produced further it must be separated from the reactants (oxygen and nitrogen) and the by-products of the reaction (acetic acid and water). In order to determine the most economic and efficient method of separation, different processes have been evaluated [17 - 20]. Lloyd Berg investigates the dehydration of acrylic acid using certain organic compounds as the agent in extractive distillation [18]. Extractive distillation is effective technic to separate close boiling compounds or azeotropes, but still requires an entrainer. The extractive agent (entrainer) is introduced near the top of the column and its presence alters the relative volatility of the compounds to allow a greater degree of separation. The main disadvantages in this case are: the added cost of the entrainer and additional equipment (usually a distillation column) for its regeneration. A method of azeotropic distillation for producing highly pure acrylic acid by Kazuhiko Sakamoto et al. has been proposed [17]. In this case water is added to the reaction product to obtain an aqueous solution of the product. An azeotrope solvent is further added in the solution thereby removing by-products through the azeotrope formation. Thus, water and the azeotrope solvent are separated from a tower top and acrylic acid from a tower bottom. The same disadvantages as in the previous case of extractive distillation may be given. The same disadvantages as in the previous case of extractive distillation (the added cost of solvent and keeping the number of distillation towers) may be given. Another commonly used method for producing AA is by including liquid-liquid extraction to allow better separation of organic components from water [21, 22].

In this invention a simple pathway to produce glacial-grade AA has been developed. The main idea is to avoid expensive and complicated processes of extractive or azeotropic rectification, as well as liquid-liquid extraction. To separate light non-condensable gases the phase separator operation at low temperature of 263 K has been used. In order to obtain optimal operating conditions the sensitive analyses (see part ‘Light gas separation”) of temperature and pressure have been made. The operating conditions in the phase separator are selected to ensure minimal losses of AA and acrolein with the gas mixture leaving the separator. On the other hand, the obtained liquid mixture must allow further separation and production of 99.9 mol % AA by conventional distillation. The liquid fraction obtained contains mainly AA and small amounts (5 mol %) of acrolein. Thus, the stages of separation of light non-condensable components from the total mixture is completed.

The final separation process contains two series-connected distillation columns. In the first column, acrylic acid with a purity of 99.9 mol % as a bottom product is obtained. The top product is a mixture of water and acrolein, as well as small amounts of acrylic acid and traces of unreacted propylene. This stream was fed to the second distillation column, where pure water with a concentration of 98.2 mol % was obtained as the bottom product, and acrolein approximately 90 mol % as the top product. The obtained acrolein is returned to the reactor section for reuse. Therefore, main objectives of this investigation are:

- To simulate a complete process for acrylic acid manufacturing by partial propylene oxidation.
- To develop and optimize the separation sections and operating conditions on acrylic acid plant.

MODEL DESCRIPTION

Thermodynamic requirements

Selection of the proper method for estimating properties is one of the most vital steps that will affect the rest of the simulation. Therefore, it is important to carefully consider the choice of the correct property method to estimate the different properties. Since the whole production process is a combination of chemical reaction, distillation, condensation, etc. in all cases the mathematical description should include both mass transfer processes and chemical processes.

Fluid phase equilibrium

Mass transfer processes associated with the heating and cooling processes, condensation, distillation etc. represent bidirectional diffusion through vapor/liquid interphase surface. In other words, the correct description of the fluid phase equilibrium is necessary. In this study base of the K-value methods the required thermodynamic data for phase equilibrium were obtained. The NRTL-HOC method was selected to describe the phase equilibrium behavior of this process with NRTL to account for non-ideal liquid behavior and HOC (Hayden-O'Connell) to account for possible associate behavior of acrylic acid and acetic acid in vapor phase [23]. This property method also incorporates the chemical theory of dimerization which is a possible phenomenon to form in this process. The liquid-phase activity coefficients are well represented by the NRTL equation. The NRTL binary interaction parameters (BIPs) were obtained from both literature data [21, 24] and data base of ChemCAD. The UNIFAC thermodynamic property model was employed to estimate the missing binary parameters.

Reaction kinetic

This is normally done as a standard process involving two reactors in series, utilizing two separate catalysts. In this arrangement, the first reactor converts the propylene to acrolein while the second reactor completes the conversion from acrolein to AA. Each reaction step usually takes place over a separate catalyst and at different operating conditions.

Research into partial oxidation of propylene to acrolein in the past decades has been focused on more fundamental understanding of the mechanisms at molecular levels, particularly the events that take place on the surface of catalysts [26, 27]. The current understanding of the mechanism and kinetics of the selective catalytic oxidation of propylene to acrolein is based on extensive investigations with bulk mixed metal oxides that primarily employed bulk Bi–Mo–O catalysts [27, 28]. Based on the literature [26 - 28], the chemical reactions taking place in first Reactor are as follows:

$$C_3H_6 + O_2 \rightarrow C_3H_4O + H_2O,\ Extent - 79\ \% \tag{1}$$

$$C_3H_6 + \frac{3}{2}O_2 \rightarrow C_3H_4O_2 + H_2O,\ Extent - 6\ \% \tag{2}$$

$$C_3H_6 + \frac{5}{2}O_2 \rightarrow C_2H_4O_2 + H_2O,\ Extent - 12\ \% \tag{3}$$

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O,\ Extent - 3\ \% \tag{4}$$

This reaction scheme is carried out using a α - $Bi_2Mo_3O_{12}$ catalyst [27].
Acrolein oxidation constitutes the second step of a two-step process of propylene oxidation to acrylic acid. The chemical reactions taking place in second Reactor using the VMo_3O_{11} catalyst are as follows [25 - 27]:

$$C_3H_4O + \frac{1}{2}O_2 \rightarrow C_3H_4O_2,\ Extent - 85\ \% \tag{5}$$

$$C_3H_4O + \frac{7}{2}O_2 \rightarrow 3CO_2 + 2H_2O,\ Extent - 15\ \% \tag{6}$$

The kinetics for the reactions presented above is described by the following rate expression:

$$r_i = K_i \exp\left(\frac{-E_i}{RT}\right)\prod\nolimits_j P_j \tag{7}$$

Set of parameters are borrowed from experimental data [25, 27]. The results for the activation energy (E_i), the frequency and factor (K_i) and partial pressure (P_i) have been obtained at a constant catalyst loading. Thus, using these results the influence of catalyst on the reaction kinetic was taken into account.

PROCESS DESCRIPTION

In Fig. 1 the flow-sheet diagram and the detailed process description from raw materials to AA as final product are presented.

Preparation of the raw materials

The first part of the flowsheet is to prepare the raw materials for the main process. The initial feed streams 1 and 2 are respectively air and acetylene flow with environmental temperature 25^{o}C and pressure 1 atm. The flow rates of the two streams are chosen in correspondence with the stoichiometry of the reactions. Thus, the air flow rate is 39600 kg/h and propylene flow rate is 5000 kg/h. Since the chemical reactions run at increased pressure and temperature, the

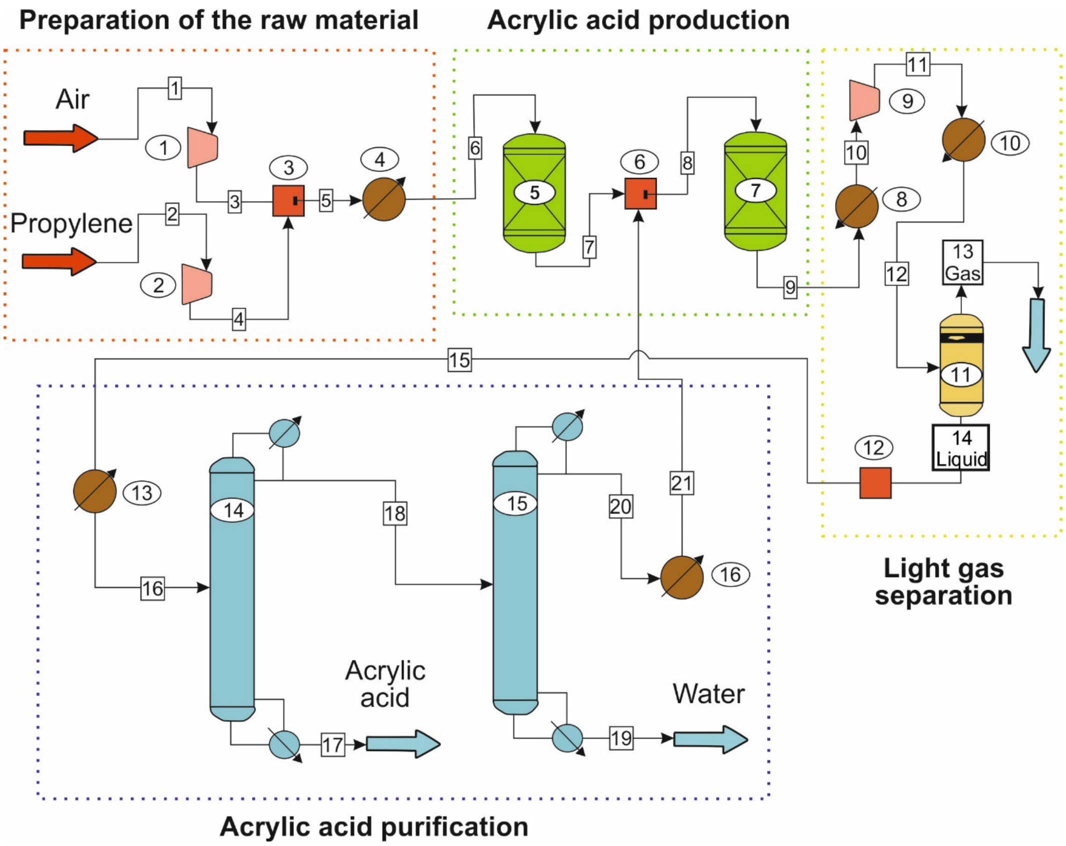

Fig. 1. Flow-sheet diagram.

preparation of the raw materials involves compressing and heating to the necessary temperature. The initial raw materials propylene and air are compressed in two separate compressors: for air 1 and for propylene 2. Because compressing is an exothermic process, the pressure rising in the compressors 1 and 2 leads to an increase in temperature. So during the compression process the temperature of the air stream is increased from 25 °C to 253.471 °C and the acetylene stream from 25 °C to 113.299 °C. Thus, the compressors are preheaters in regard to the raw materials. In the mixer 3 a homogeneous mixing of the air and propylene streams is carried out. Since the temperature of the two gas streams (3 and 4) are different (253.471 °C for the air and 113.299 °C for the propylene) and base on the heat balance of the mixer 3 the final temperature of the gas mixture in stream 5 is 225.547 °C. According to literature the optimal temperature for running the basic chemical reactions is 300 °C [25 - 27]. Therefore, before entering in reactor 5 the gas mixture from the mixer 3 is heated from 225.547 °C to 300 °C in the heat exchanger 4.

Acrylic acid production

In the reactors 5 and 7 the main production of acrylic acid is carried out. In the reactors the catalytic propylene oxidation and all accompanying chemical reactions are carried out.

Regarding the use of two types of catalyzers and the different working conditions, the chemical reactions are distributed in two apparatus:

- In the first reactor (number 5) reactions from (1) to (4) witch refer to the acrolein formation using the first type of catalyst are carried out;
- In the second reactor reactions 5 and 6 associate with the catalytic acrolein oxidation using the second type of catalyzer take place.

In Table 1 the composition of the products obtained in reactor 5 is presented.

It can be seen that in the reactor 5 a very small quantity of acrylic acid and about 7.77 mol % acrolein are obtained. Stream 7 leaving reactor 5 is mixed with stream 20 going out from the top of the distillation column 12. Stream 20 is acrolein recycling stream

Table 1. Composition of the products obtained in reactor 5.

Stream No	Reactor 5
Name	Component mole %
Water	8.171690
Carbon Dioxide	0.001415
Acetic Acid	0.001395
Acrylic Acid	7.585336
Acrolein	1.321040
Propylene	0.088057
Oxygen	5.958204
Nitrogen	76.872855

containing 90.48 mol % acrolein. In mixer 6 two streams 7 and 20 are mixed. Thereafter, the obtained mixture (stream 8) containing 8.49 mol % acrolein enters in reactor 7, where the catalytic oxidation of acrolein to AA is carried out.

Light gas separation

The first separation step for the products obtained in chemical reactor 7 is light gases separation. This is done through initial cooling of the gas mixture stream 9 in heat exchanger 8. Then stream 10 is compressed to pressure $P=30$ *atm* in compressor 9 and then stream 11 is cooled to temperature -10 C in heat exchanger 10 ($= 30$ *atm* and $T = -10$ *°C* are necessary for the optimum work conditions of separator 11 - see part “Light gas separation”). In separator 11 the liquefaction of vapor components is carried out. Thus, the light gases such as nitrogen and oxygen, carbon dioxide are separated in stream 13.

Acrylic acid purification

The liquid mixture leaking from separator 11 reduces its pressure from 30 to 1 atm by passing through pressure relief device 12. Then the stream 15 is heated in heat exchanger 13 to temperature 105 °C. This temperature is required for obtaining the vapor-liquid steam 16 used as feeding for first distillation column 14. In this column as bottom product (Stream 17), acrylic acid with purity 99.9 mol % is obtained. The distillate of column 14 (Stream 18) is a mixture of water, small quantities acrolein, acrylic acid and traces of propylene. Stream 18 is fed in second distillation column 15, where the water with purity of 98.2 mol% as a bottom product is obtained. The top product of column 18 is acrolein approximately 90 mol % and water. For recycling of acrolein stream 20 after heating in heat exchanger 16 is fed through mixer 6 in reactor 7. Thus, from 5000 kg/h of propylene and 39600 kg/h of air 82299.29 kg/h of acrylic acid with a purity of 99.9 mol% and 2250.14 kg/h of water with a purity of 98.2 mol% are obtained. During the process, 34050.57 kg/h of light gases composed mainly of nitrogen and oxygen are released.

RESULTS AND DISCUSSION

As it was mentioned, the main idea of this investigation is developing a new method for separation and purification of the acrylic acid obtained in chemical reactors for catalytic oxidation of propylene. Our concept is initially from the gas mixture leaving reactor 7 to be separated the light non-condensed compounds (nitrogen, oxygen, carbon dioxide) through cooling down the mixture and liquefaction of the heavy compounds (water, acrylic acid, acetic acid, acrolein). It is carried out at appropriate working conditions in separator 11. The second step is separation of the liquid mixture leaving separator 11 and obtaining pure acrylic acid and pure water as bottom products in rectification columns 13 and 14. In this regard, the main investigations are associated to parts “Light gas separation” and “Acrylic acid purification” of the process flow-sheet. Therefore, the sensitive analyses for the complex influence of the kay parameters in different apparatus are carried out.

Light gas separation

Sensitive analyses of separator (condenser) 11

Separator 11 is a condenser where the non-condensed gases such as nitrogen, oxygen, carbon dioxide are separated from condensable compounds - acrylic acid, acetic acid, and acrolein. The target compounds, which should not be separated with the flow of light gases, are acrylic acid and acrolein. Their presence in the mixture of light gases is identified as process losses. Therefore, the influence of the temperature and pressure on the loss of key compounds: acrylic acid and acrolein is investigated.

Acrylic acid losses

The influence of the temperature on the loss of key compounds at a pressure 1 atm in the gas flow leaving the condenser 11 is shown in Fig. 2.

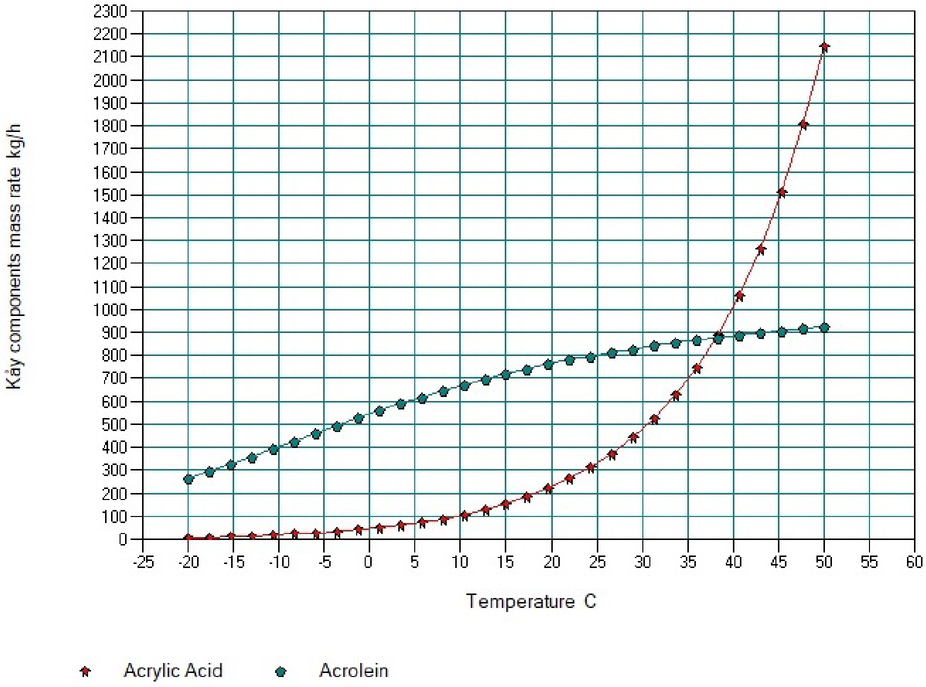

Fig. 2. Influence of the temperature on the loss of key compounds at a pressure of 1 atm.

Fig. 2 shows a significant effect of temperature on the loss (increase in the flow rate of acrylic acid in stream 13) of the acrylic acid. This influence has an exponential character at temperature above 1°C. As a result, it is unacceptable at pressure 1 atm to work at temperature higher than -10 °C. At a temperature -10 °C the acrylic acid loss is 17.89 kg/h, at room temperature (20 °C) this loss is 220.23 kg/h.

The acrylic acid loss in stream 13 as a function of pressure at temperature T = - 10 °C is shown in Fig. 3. The curve in Fig.3 passes through minimum at pressure about 30 bar. It means that at this temperature the optimum pressure of 30 bar can be chosen.

Acrolein losses

Fig.2 shows that acrolein loss at temperature up to 30 °C is much larger than this of the acrylic acid. For example, at temperature T = - 10 °C the loss of acrylic acid is 17.89 kg/h and of acrolein is 394.06 kg/h. The influence of the temperature on acrolein flow rate is analogical with this of the AA. As the temperature rises, acrolein losses increase, but not as fast as acrylic acid.

The influence of the pressure on acrolein losses at T = -10 °C is presented in Fig. 4. As the pressure rises reduces the loss of acrolein, the most significant effect is up to a pressure of 20 bar. After 20 bar the flow rate of acrolein changes slightly. The curve passes through a minimum at a pressure of about . Therefore, the pressure of 30 bar will be suitable

with regards to acrolein loss.

The complex influence of the temperature and pressure on the acrolein loss is shown in Fig. 5. In this case, the ranges of variation of these two parameters are in accordance with the results of previous sensitive analyses (see Figs. 2 - 4).

In conclusion, due to the much greater loss of acrolein than AA, it is appropriate to optimize the separator 11 for acrolein losses. Thus, at a pressure greater than 30 bar the acrylic acid loss begins to increase. Therefore, as optimal operating conditions for the separator 13 the temperature of T = - 10 °C and the pressure of 30 bar have been selected. In this case the loss of target products is minimum – acrolein 31.48 kg/h and acrylic acid – 1.75 kg/h.

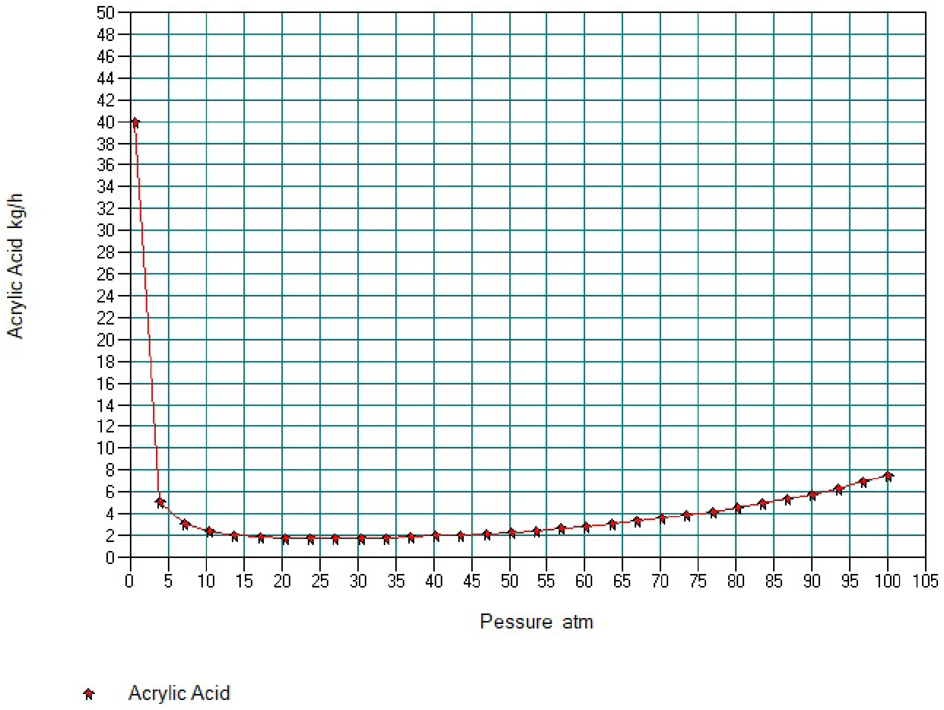

Fig. 3. Influence of the pressure on the loss of acrylic acid at a temperature of -10 °C.

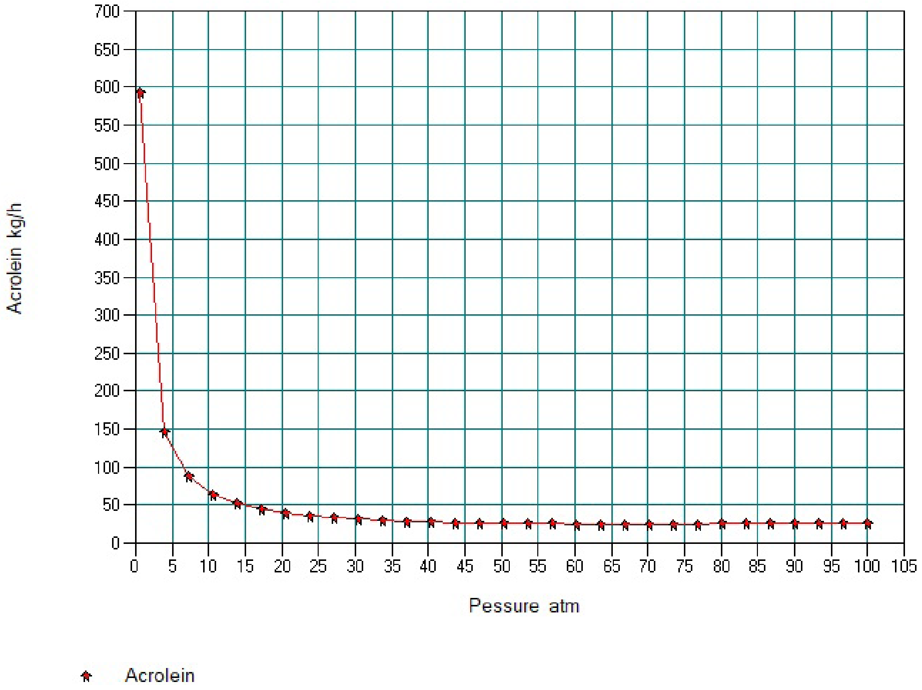

Fig. 4. Influence of the pressure on the loss of acrolein at a temperature of -10 °C.

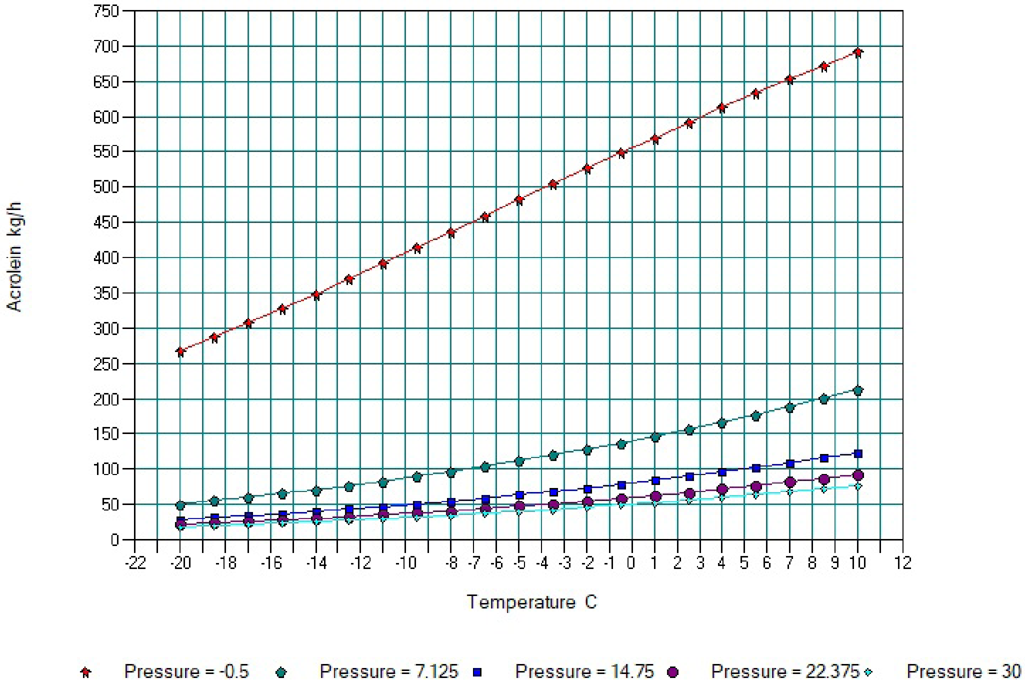

Fig. 5. Complex effect of temperature and pressure on acrolein loss.

Acrylic acid purification

Fluid phase equilibrium

The composition of the streams 13 and 14 leaving the separator 11 is shown in Table 2.

The Table 2 shows that the non-condensable fraction (light gasses) contains mainly nitrogen and oxygen and very small amounts of water and acrolein. The obtained liquid fraction (condensable fraction) contains mainly water, acrylic acid and small amounts (5 mass %) of acrolein. In Fig. 6, the vapor-liquid equilibrium of the triple system water-acrylic acid-acrolein is presented. To construct a triangular diagram of the triple system the residual curves maps method is used.

One of the methods for separating such a mixture is rectification. Fig. 6 shows that the most volatile component is acrolein followed by the water and the heaviest compound is acrylic acid. This system forms a binary azeotrope between water and acrolein with a composition of 8.3 mol % water and 91.7 mol % acrolein, which has a boiling point at 51.99 °C. This azeotrope cannot be destroyed by conventional rectification. In this sense, the azeotrope must be treated as a different compound of the system. Thus, the azeotrope will be the most easily volatile component and will accumulate in the top of the column. To separate this three-component liquid mixture by distillation more than one distillation column is required. Following the rule of trump for chemical engineers, the first distillation column separates the compounds that are in the largest quantities [29].

Table 2. Composition of the streams 13 and 14.

Stream No	13	14
Name	GAS	Liquid
	Component mole %	Component mole %
Water	0.009820	46.139053
Carbon Dioxide	0.001686	0.003130
Acetic Acid	0.000001	0.007837
Acrylic Acid	0.002057	45.217675
Acrolein	0.046824	7.664888
Propylene	0.098800	0.833206
Oxygen	6.923983	0.016632
Nitrogen	92.916828	0.117579

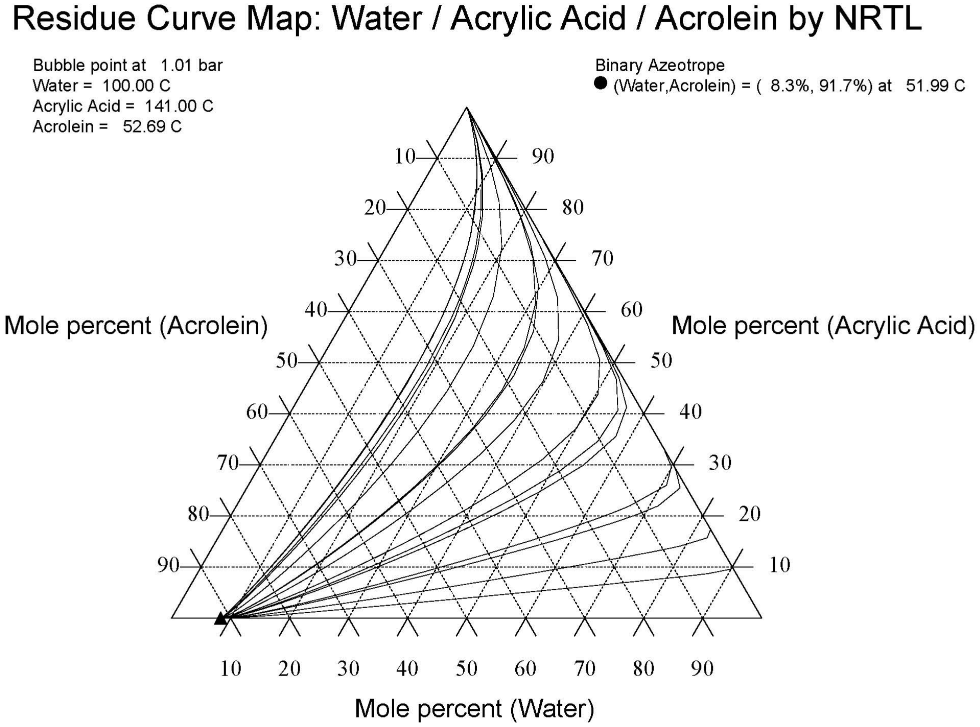

Fig. 6. Residue curve maps for the system water/acrolein/acrylic acid.

In our specific case, these are water and acrylic acid. Therefore, water and acrylic acid are separated in distillation column 13. Since AA has the highest boiling point (the nonvolatile component), it will separate at the bottom of column 13. Acrolein and the binary azeotrope are more volatile than water, so they will accumulate at the top of column 13.

In order to simulate the distillation process in both columns (13 and 14) the SCDS module in ChemCAD software is used. SCDS is a rigorous multi-stages vapor-liquid equilibrium module which simulates any single column calculation. By this module columns with unlimited stages, five feed streams, and four side products can be simulated. SCDS can simulate rigorous distillation of two-phase or three-phase non-ideal K-value chemical systems. It uses a Newton-Raphson convergence method with simultaneous correction and calculates the derivatives of each equation rigorously, including the $\partial K/\partial x$ (derivative of K-value with respect to composition) term which is significant in chemical system simulation [30].

In order to be obtained the optimal operation conditions of distillation columns, sensitive analyses were carried out. In this work the sensitive analyses were performed on the parameters exerting the most significant influence on the yield of acrylic acid. These parameters are: number of stages, a feed stages location, and an influence of the reflux ratio.

Sensitive analyses of column 14

Distillation column 14 is intended for the production of glacial-grade acrylic acid at the bottom of the column. It is possible because the acrylic acid is the highest boiling point compound and it is contained in large quantities in the stream 14 (see Table 2). All simulations showed that 99.9 mol % acrylic acid at the bottom of column 14 was obtained. In all cases, a certain amount of acrylic acid is accumulated into the distillate of the column. This amount represents a loss of acrylic acid. Therefore, sensitive analyses of column 14 are referred to minimizing these losses.

Sensitive analysis of Number of stages

During the sensitive analysis for column 14 the number of stages was changed from 10 to 30 and the results are shown in Fig. 7.

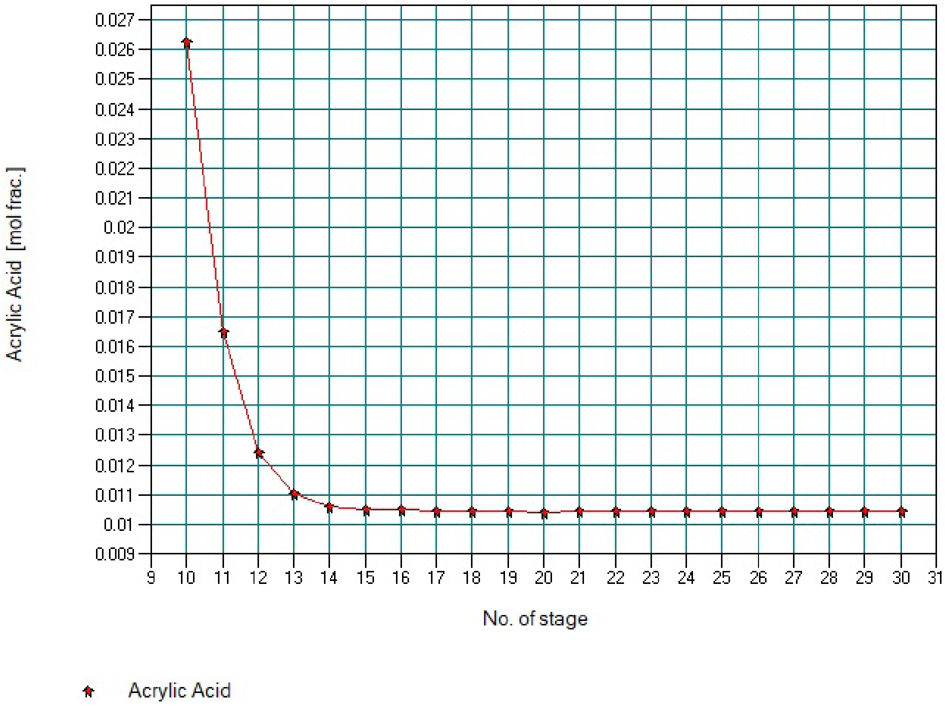

Fig. 7. Effect of number of stages on the acrylic acid concentration (mass parts) in the distillate.

The Fig. 7 shows the change in the concentration (in mass parts) of acrylic acid in the distillate, depending on the number of stages. With increasing number of stages the concentration of acrylic acid in the distillate decreases exponentially, and at a number greater than 14 the concentration practically does not change. It is better to keep the number of stages to a minimum in terms of the cost of the distillation column as well as the operating costs. Thus. the optimal number of stages is 14.

Sensitive analyses of feed stages location

The mathematical model in the SCDS module in CHEMCAD provides counting the number of stages from the top to the bottom of the column. Thus, the first stage is the reflux condenser and the last stage is the column evaporator. If we set 14 degrees as optimal for column 14, then the actual number of stage inside the column 14 will be from 2 to 13. Therefore, during sensitive analysis, the feed stage location is changed from 2 to 13. The result is shown in Fig. 8.

The Fig. 8 shows that the lowest concentration of acrylic acid in the distillate is obtained if the feed stage location is *8 (X = 0.0090 mass part)* - to *10 (X = 0.0131 mass part)*. Thus, stage number 9 as optimal feed stage location is selected.

Sensitive analyses of the reflux ratio

The Fig. 9 shows the change in the concentration of acrylic acid in the distillate when the reflux ratio (*R*) varies from 0.15 to 10.

The Fig. 9 shows that with increasing R the concentration of acrylic acid in the distillate decreases very rapidly and at $R > 2$ it almost does not change. Therefore, $R = 2$ is chosen as the optimal reflux number. Thus, the optimal result obtained during sensitive analyses of column 14 is: number of stages - 14, the feed stages location - 12 and the reflux ratio - 2.

Sensitive analyses of column 15

A distillation column 15 is used to separate the distillate coming from column 14 (stream 18). Table 3 shows the composition (in mass parts) of stream 18.

The stream 18 contains mainly water and acrolein, small amounts of propylene and acrylic acid. The purpose of column 15 is to separate the water from stream 18 as a bottom product. Thus, the distillate (top

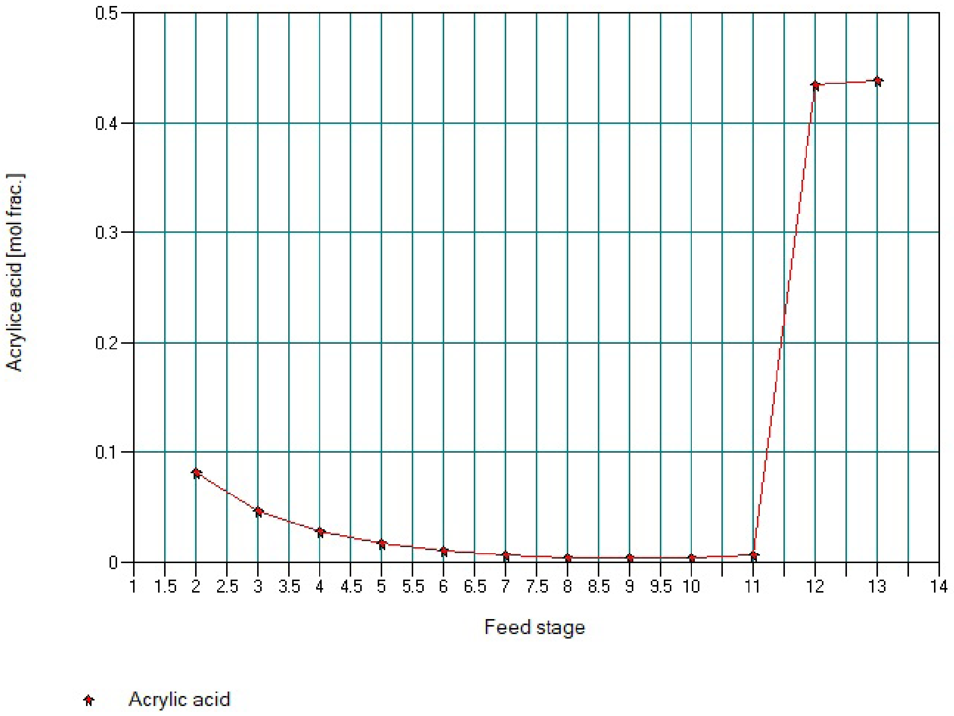

Fig. 8. Acrylic acid concentration (mass parts) in the distillate according to the feed stages location.

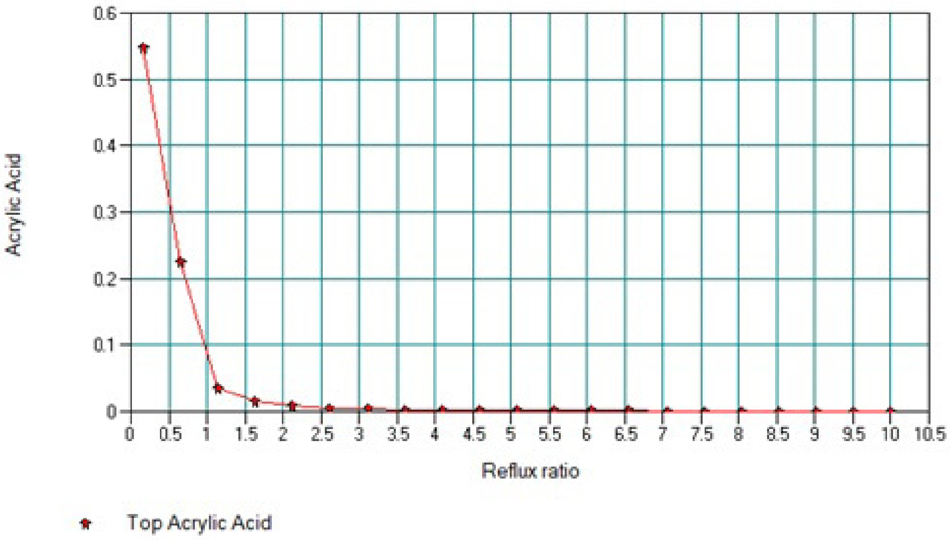

Fig. 9. Effect of reflux ratio on the acrylic acid concentration (mass parts) in the.

Table 3. Composition of stream 18.

Stream No	18
Name	Component mole %
Water	83.178622
Carbon Dioxide	0.005647
Acetic Acid	0.001614
Acrylic Acid	1.239334
Acrolein	13.829380
Propylene	1.503313
Oxygen	0.030008
Nitrogen	0.212143

Table 4. Composition of the streams 19 and 20.

Stream No	19	20
Name	Component mole %	Component mole %
Water	98.409611	7.389998
Carbon Dioxide	0.000000	0.033749
Acetic Acid	0.001939	0.000000
Acrylic Acid	1.488398	0.000000
Acrolein	0.100000	82.146066
Propylene	0.000029	8.983578
Oxygen	0.000000	0.179327
Nitrogen	0.000000	1.267755

product) of column 15 will contain mainly acrolein, very small amounts of propylene and acrylic acid. This distillate is cooled in the heat exchanger 16 and thereafter mixing with stream 7 in the mixer 6 and returned to the reactor 7 to recycle the acrolein. Therefore, the target product of the distillation column 15 is the separation of pure water as a bottom product. The optimization involves the accumulation of as little water as possible in the distillate. Thus, sensitive analyses of column 15 were made with respect to the water content of the distillate. For column 15, sensitive analyses were performed in the same manner as for column 14. The following optimal results were obtained: number of stages - 6, the feed stages location - 13, the reflux ratio - 3. Thus, results obtained for the composition of top (stream 19) and bottom (stream 20) products of column 15 are shown in Table 4.

CONCLUSIONS

The process for a glacial-grade AA production by gas partial oxidation of propylene has been simulated. The design of the flowsheet includes all necessary technological operations and actions to receive the key components obtained from the partial oxidation of propylene. This study involved more investigation of recover acrylic acid from the gaseous reactor effluent rather than native reaction kinetic characteristics. A new simple procedure for further separation process of reactor products via condensation and conventional distillation has been developed. The sensitive analyses are incorporated to solve an optimization problem formulating with objective functions:

- to separate light non-condensable gases such as nitrogen, oxygen carbon dioxide, etc.;
- to obtain a glacial-grade acrylic acid such as bottom product in the first distillation column;
- to maximize water flow purity at the bottom of second distillation column and recovery of unreacted acrolein in top stream of the same column.

The first step to divide the reactor products is to separate the light non-condensable gases from the hot gas mixture. The optimum temperature of 263 K and the pressure of 30 atm in the condenser separator have been obtained. The second step is to obtain glacial-grade acrylic acid and water in two series-connected conventional distillation columns. The influences of the number of stages, the feed stages location, and the reflux ratio over the objective function were investigated. To obtain glacial-grade acrylic acid as the bottom product of the first distillation column optimal operating conditions: number of stages - 14, the feed stages location - 12, and the reflux ratio - 2 have been found. The present investigation shows that number of stages 6, the feed stages location - 3, and the reflux ratio - 3 are the optimal for the second distillation column. Thus, from 5000 kg/h of propylene and 39600 kg/h of air,8299.29 kg/h of acrylic acid with a purity of 99.9 mol % and 2250.14 kg/h of water with a purity of 98.2 mol % are obtained. During the process, 34050.57 kg/h of light gases composed mainly of nitrogen and oxygen are released. The developed stimulation model enables better understanding and study of the acrylic acid production via gas partial oxidation of propylene.

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