

PROCESS SIMULATION STUDY OF ETHYL ACETATE REACTIVE DISTILLATION COLUMN BY HYSYS[®] 3.2 SIMULATOR

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ABSTRACT:- In this paper, reactive distillation column for the production of ethyl acetate from ethanol and acetic acid has been simulated by the simulator tool of HYSYS. This reactive distillation is a promising operation whereby reaction and separation take place within a single distillation column.

The thermodynamic properties are calculated with the Wilson, NRTL and UNIQUAC Property Package models which are available in HYSYS simulator program.

The effects of water content in feed, bottom temperature and reflux ratio on top temperature and conversion of ethanol are studied when using three thermodynamic models and three feed statuses (upper, intermediate and spilt).

The results showed that the best conditions are: bottom temperature (83-86)⁰C, reflux ratio (2-5) without water content in feed at spilt condition using Wilson as the best model. The study gives evidence about a successful simulation with HYSYS because the results are close with the experimental data of (Calvar et al)^[18].

Keywords: HYSYS Simulator, Reactive Distillation, Esterification processes, Ethyl Acetate production.

INTRODUCTION

Ethyl acetate (EtAc) is an important organic solvent widely used in the chemical industry and in the production of varnishes, ink, synthetic resins, and adhesive agents^[1,2], and can produced directly from ethanol (EtOH) and acetic acid (HAc) under an acidic condition^[3]. A key issue in the production of (EtAc) is the low conversion from the reaction. As a result, heavy capital investments and high energy costs are inevitable. The reactive distillation is a very attract way to reduce these investments and energy costs^[2]. Reactive distillation (RD) is the combination of reaction and distillation in asingle vessel and the advantages like improved selectivity, increased conversion, better heat control, effective utilization of reaction heat, scope for difficult separations and the avoidance of azeotropes can be realized by application of reactive distillation^[4]. Conceptually, a RD column has three basic sections: rectifying section on the top, reactive section in the middle, and the stripping section at the bottoms^[1]. Succeeding researches on this reactive distillation have been reported on either steady-state simulations (e.g. Neson, 1971^[5] ; Kinoshita and

Holland , 1977 ^[6] ; Simandl and Svrcek,1991 ^[7] ; Giessler, 2001 ^[8]), dynamic modelling (e.g. Alejski and Duprat, 1996 ^[9] ; Krzysztof, 1996 ^[10] ; Kuan and shih, 2007 ^[2]), operation and control (e.g. Vora and Daoutiedis,2001 ^[11] ; Georgiadis et al. 2001 ^[12]), single column experiment (e.g. Kloker et al., 2004^[13] ; Kenig et al.,2001 ^[14]), vapor-liquid equilibria (e.g. Calvar et al., 2005 ^[15]), and reaction kinetics and operation (e.g. Kirbaşlar et al., 2001^[16] ; Hangx et al., 2001^[17] and finally Calvar et al., 2007 ^[18]), which has been simulated in this paper. The objective of this paper is to present a systematic approach for analysis the design and operation of reactive distillation process by HYSYS simulator. First, appropriate models and their parameters are validated. Second, the validated models are employed to obtain relationships between variables that have a large impact on the design and operation of the process. Finally, the obtained relationships are employed to analysis the reliability and efficiency of design and operation of the reactive distillation columns.

HYSYS PROCESS SIMULATOR

HYSYS is a process simulation environment designed to serve many processing industries especially oil and gas refining. Rigorous steady state and dynamic models for plant design, performance monitoring, troubleshooting, operational improvement, business planning and asset management can be created using HYSYS. The built-in property packages in HYSYS provide accurate thermodynamic, physical and transport property predictions for hydrocarbon, non-hydrocarbon, petrochemical and chemical fluids. They are divided into five basic methods {equations of state (LKP, PR, SRK and their modifications) for rigorous treatment of hydrocarbon systems, semi-empirical models (Chao-Seader and Grayson-Streed) and vapour pressure models (Antoine, Braun k10, Esso K) for the heavier hydrocarbon systems, activity coefficient models (Margules, UNIQUAC, Van Laar, NRTL and their modifications, etc.) for chemical systems and finally miscellaneous (special application) models (Amines and steam packages)}. Proper use of thermodynamic property package parameters is key to success simulating any chemical process. The database consists of an excess of 1500 components and over 16000 fitted binary coefficients. If a library component cannot be found within the database, a comprehensive selection of estimation methods is available for creating fully defined hypothetical components.^[19,20]

The calculation method for distillation in HYSYS is done to a high standard in accordance with the matrix method. A quick convergence and short simulation time is therefore guaranteed. In most cases ,the user need not be concerned with the details of the internal calculation, this is done automatically by HYSYS , and the following six basic steps are used to run a flowsheet simulation in HYSYS are:^[21]

1. Selecting components.
2. Selecting thermodynamics options.
3. Creating a flowsheet.
4. Defining the feed streams.
5. Input equipment parameters.
6. Running the simulation & Reviewing the results.

Figures (1 and 2) show the schematic diagram of ethyl acetate Reactive distillation column and the residue curve map of (HAc–EtAc–H₂O) system respectively, which have been constructed using HYSYS.

Reactive distillation is represented by HYSYS using three phase distillation template. The key difference between using the standard column templates and their

three phase counterparts lies on the solver that is used. The default solver for three phase columns is the sparse continuation solver which is an advanced solver designed to handle three phase, non ideal systems, that other solvers cannot. When using the three phase column template some additional specifications can be required when compared with the standard (binary system) column setups. It requires some expertise to setup, initialize, and solve three phase distillation problems. Additional modeling software applications such as DISTIL, use residue curve maps and distillation region diagrams to determine feasible designs, and can greatly assist in the initial design work^[22].

Reactive distillation column used in the production of ethyl acetate has been simulated using HYSYS simulator. The operation conditions of the different runs have been divided in two setups depending on the feed was introduced into the column as a mixture of reactants or the reactants were fed separately.

First setup. The process of reactive distillation was first analyzed with one feed, formed by ethanol and acetic acid. This feed was introduced in the column in different sections (upper and intermediate feed), and with different water content in feed.

Second setup. The reactants, ethanol and acetic acid, were fed into the column separately. Acetic acid was always introduced in the higher section, because it is less volatile than ethanol, see figure (1).

REACTION KINETIC

The homogenous and heterogeneous catalyzed esterification kinetics have been studied by several workers, such as Kirbaşlar et al.^[16] and Hangx et al.^[17] but they do not take into account the activity coefficient of the compounds in the mixture compare with Calvar et al.^[18], and according to the Calvar et al.^[18] work, the homogeneous reactions (esterification or hydrolysis) are catalyzed by the acetic acid according to the following equation:



Calvar et al.^[18] used the following equation (which is taken from Pöppken et al.^[23]) to fit their experimental data:

$$r = n_o \frac{dx}{dt} = a_{HAc}^\alpha (K_1 a_{HAc} a_{EtOH} - K_{-1} a_{EtAc} a_{H_2O}) \dots\dots\dots (2)$$

Where: α can take the values of (0.5 or 1) when the autocatalysis mechanism is via the solvated protons of the dissociated acid or via the molecular acid, respectively. Activities were calculated using ASOG^[24] and UNIFAC^[25] methods, to calculate activity coefficients, and assuming an ideal behavior. Calvar et al.^[18] used the Arrhenius' law,

$$k_i = K_i^0 \exp(-E_{a,i}/RT) \dots\dots\dots (3)$$

to express the temperature dependence of the rate constants. They calculate the pre-exponential factors and activation energies of esterification and hydrolysis using $\alpha = 1$, liquid phase activities which is calculated by ASOG and UNIFAC, and the estimated parameters k_1 and k_{-1} . The Arrhenius diagrams for both fits are presented in figure (3), and table (2) summarizes the kinetic parameters using ASOG and UNIFAC models and $\alpha=1$, which are used in this study.

RUSULTS AND DISCUSSION

The reactive distillation column used in the production of ethyl acetate has been simulated using HYSYS® 3.2 simulator. There are many variables influence this production such as water content in feed , bottom temperature , and molar reflux

ratio (RR) . The influence of each variable on top temperature and conversion of ethanol can be study by using different thermodynamic models to find the best operating conditions for production of ethyl acetate .

EFFECT OF WATER CONTENT IN FEED

Figures (4 to 9) show the effect of water content in feed on top temperature and conversion of ethanol when using different thermodynamic models. It is noted that the impact of the percentage of water inside of the mid-tower with nutritious is almost non-significant on the temperature at the top of the tower and applicable to each model (Wilson, NTRL, UNIQUAC), because of increasing acetic acid quantities according to chemical reaction, so it will accumulate at the tower bottom as a result of its high normal boiling point. While the effect will be observed and a relatively large proportion of the conversion, and that the greatest impact is in UNIQUAC at (20%) , and the change is decreasing with increasing water content according to chemical reaction, in which the backward reaction its will increasing. The impact of increased water content in the case of split feed, top temperature as well be imperceptible, and the reason behind is not affected by the temperature at the top of the tower is that the home by quantity of water will cool the vapor rising to (70⁰C) and the increase in the rate of ingress of water will lead to decrease in temperature inside the tower, leading to collapse of the tower work later. While the impact of water inside the tower in the case of the split feed on the conversion within the medium levels of impact and that the greatest impact was at a water content is (70%) in the case of Wilson . It is also clear here that the highest impact in the case of increasing water content for the upper feed for they do not exceed (1.5%) for the temperature at the top of the tower, it is possible to neglect this effect. While the impact of increased water content in the case of entry of the upper feed conversion ratio to be clear and large and are between (15-22% down), and because increased water content, working to alleviate the acid, which operated as a catalyst in such reactions. In spilt feed form, we achieved a higher conversion compared with the other feed forms (top and intermediate) because of we provide a large lag time for reaction to take place.

EFFECT OF BOTTOM TEMPERATURE

Figures (10 to 15) show the effect of bottom temperature on top temperature and conversion of ethanol at different thermodynamic models. The increase in temperature of (80-95)⁰C for the reboiler is within the specifications of the design and operational conditions of the tower, has been observed that increasing the temperature of the reboiler with not much on the temperature at the top of the tower, because of acetic acid an reached a normal boiling point and that will lead to an raising the acetic acid vapor to top of tower. But the impact of the increase in temperature bottom of the tower on the conversion is typically non-linear, where the conversion begins to decline with increasing temperature of the bottom of the tower for the all models (fluid package) and the rate nearly (15%), but after starting the proportion at (89⁰C) shift upward, but at a lower rate of approximately (7-8%) because of increasing bottom temperature, firstly will accelerate the backward reaction, decreasing an ethanol conversion, until to (89 °C) that will be increase the potential energy of acetic acid and can be seen the increasing of ethanol conversion. Consideration of the impact remains widget (95⁰C) temperature of the bottom of the tower on the top temperature

of the tower for split feed condition within the natural production of ethyl acetate at temperature (71⁰C). Effect of temperature, while the bottom of the tower on the conversion, the temperature here is a very important and control must be taken into account, and work to varying thermal rather low (T = 85-87⁰C) is the best, because it allow us to get the best productivity mate of the terms of the conversion here between the (72-78%). Almost greatest increase in temperature at the top of the tower in the case of the upper feed due to increased temperature at the bottom of the tower is (2%), the low note and in all fluid packages, while we note the behavior of the conversion decreasing with increasing temperature at the bottom of the tower at (11.5%), and temperatures higher than (90⁰C) we note that the conversion begins increase but at a very low (1.5%).

EFFECT OF MOLAR REFLUX RATIO (RR)

Figures (16 to 21) show the effect of molar reflux ratio (RR) on top temperature and conversion of ethanol at different thermodynamic models. The increasing of (RR) leads to cool the tower (reducing top temperature) by limiting levels because of we do not apply subcooling to condenser. Referrer proportion of the effect of changing the temperature at the top of the tower in case of intermediate feed, we will notice in the case of the NRTL the lack of any noticeable change in temperature of the top of the tower and also the case for UNIQUAC but the difference between them that the temperature in NRTL working (68 ± 8%)⁰C, while the works UNIQUAC temperature of (67 ± 2%)⁰C, but the case is slightly different for Wilson, where it works for the extent between the latter (68-66)⁰C. While the case is completely different in the case of the conversion, the increasing of (RR) leads to increase ethyl acetate quantities which lead to increase the reverse reaction that causes decreasing the ethanol conversion, as all models are changing dramatically from RR = 2.5 to RR = 10 and after the RR = 10 begins to take form a simple change.

TEMPERATURE PROFILE OF ETHYL ACETATE REACTIVE DISTILLATION TOWER

Figure (22) shows the temperature profile of tower when using wilson model at split feed condition, the temperature increases from (71 to 75 ⁰C) when coming down from top of tower (from condenser to reboiler), except at the mid of the tower where temperature decreases because of the chemical reaction takes place at this region.

COMPARISON BETWEEN SIMULATION AND EXPERIMENTAL RESULTS

The comparison of the simulated results with experimental parameters is shown in Tables (1),(3),(4). The deviation between experimental and simulated results takes place as a result of using multi-thermodynamic models, a commercial simulator (HYSYS), and may be other thermodynamic models which are not available in HYSYS such as (UNIFAC) model can be used to describe this system. The study gives evidence about a successful simulation with HYSYS because the simulated results close with the experimental data of (Calvar et al)^[18] at the same operating conditions.

CONCLUSIONS

1. The effect of most variables on top temperature of the reactive distillation tower is almost non-significant.
2. The increase in the rate of water content in the feed will lead to decrease in temperature inside the tower, leading to collapse of the tower work later, also it will lead to alleviate the acid, which operated as a catalyst in such reactions, and as result, the production of (EtAc) is reduced.
3. The simulation results show that the best operating conditions which give the best conversion (72 – 78 %) are :
 - Bottom temperatures in the range of (85-87)⁰C .
 - Molar reflux ratio in the range of (2-5).
 - The best thermodynamic model used is Wilson in most cases.
 - The best feed is the spilt feed.

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ABBREVIATIONS

Empirical K-value model uses the Maxwell-Bonnel vapor pressure equation to calculate K-values, used for heavy hydrocarbon materials effectively at pressures below 7 bar. This model can be used to model vacuum towers.	ESSO K
<u>Non-Random Two-Liquid</u> Equation based on activity coefficient Equilibrium thermodynamic model recommended for Polar (Highly Non-Ideal Solutions).	NRTL
<u>Peng-Robinson</u> thermodynamic model to calculate K-values, based on equation of state recommended for most hydrocarbon systems.	PR
<u>Soave-Redlich-Kwong</u> thermodynamic model to calculate K-values, based on equation of state recommended for most hydrocarbon systems.	SRK
<u>Universal Quasi Chemical</u> activity coefficient equilibrium thermodynamic model recommended for polar (highly non-ideal solutions).	UNIQUAC
Zudkuvitch Jofee model is a modification of the Redlich Kwong equation of state. This model is enhanced for better prediction of vapor liquid equilibria for hydrocarbon systems, and systems containing H ₂ .	ZJ
<u>Lee Kesler Plöcker</u> Equation is an accurate general method for non-polar substances and mixtures.	LKP
Ethyl Acetate.	EtAc
Ethanol.	EtOH
Acetic Acid.	HAc
Reactive Distillation.	RD
Reflux Ratio.	RR
Activity	A
apparent activation energy (kJ mol ⁻¹)	EA,1
kinetic constant for homogeneous reaction (mol s ⁻¹)	K _i
Pre-exponential factor for homogeneous reaction (mol s ⁻¹)	k _i ⁰
mole number	N
reaction rate for homogeneous reaction (mol s ⁻¹)	R
temperature (K)	T
gas constant (J mol ⁻¹ K ⁻¹)	R
Conversion	X
parameter that takes into account the acid autocatalysis in the homogeneous reaction	A

Table (1): Typical Simulation Results Using Wilson Thermodynamic Model at ($T_{\text{bottom}} = 85\text{ }^{\circ}\text{C}$ and Reflux Ratio = 2.5).

Variables	Values
F_{HAc} (mol h ⁻¹)	3.9
F_{EtOH} (mol h ⁻¹)	3
Top Temperature (°C)	71
Conversion % (EtOH)	78
X_{D} (HAc)	0.115
X_{D} (EtOH)	0.029
X_{D} (H ₂ O)	0.228
X_{D} (EtAc)	0.628
Condenser Duty (Q _c), KJ/h	300.5
Reboiler Duty (Q _r), KJ/h	259.38

Table(2): Pre-exponential factors and activation energies of homogenous esterification and hydrolysis reactions calculated using ASOG and UNIFAC by Calvar et al. ^[18].

Parameters	ASOG	UNIFAC
$E_{a,1}$ (kJ mol ⁻¹)	41.43	53.74
$E_{a,-1}$ (kJ mol ⁻¹)	30.06	60.50
k_1^{pre} (mol s ⁻¹)	65.75	3317.28
k_{-1}^{pre} (mol s ⁻¹)	0.06	4619.43

Table (3): Experimental Data of Calvar et al. ^[18] for Ethyl Acetate reactive distillation column.

Variables	Values
F_{HAc} (mol h ⁻¹)	3.9
F_{EtOH} (mol h ⁻¹)	3
Top Temperature (°C)	70
Conversion % (EtOH)	60
xD (HAc)	0
xD (EtOH)	0.3
xD (H ₂ O)	0.148
xD (EtAc)	0.552
Internal Specification	
Column Diameter D (m)	0.05
No of Trays	3
Reactive trays	Tray No. 2
Column Height H (m)	1
Packing on trays (1 and 3)	Multiknit supplied by Tisssmetal
Reaction packing on tray (2)	Amberlyst 15 supported on Katapak-S (Sulzer Chemtech)

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Table (4): Comparison between simulated and experimental data of Ethyl Acetate reactive distillation column at; $T_{\text{bottom}} = 85^{\circ}\text{C}$, Reflux Ratio = 2.5.

Variable	experimental	Simulated
Top Temperature ($^{\circ}\text{C}$)	70	71
Conversion % (EtOH)	60	78
x_D (HAc)	0	0.115
x_D (EtOH)	0.3	0.029
x_D (H ₂ O)	0.148	0.228
x_D (EtAc)	0.552	0.628

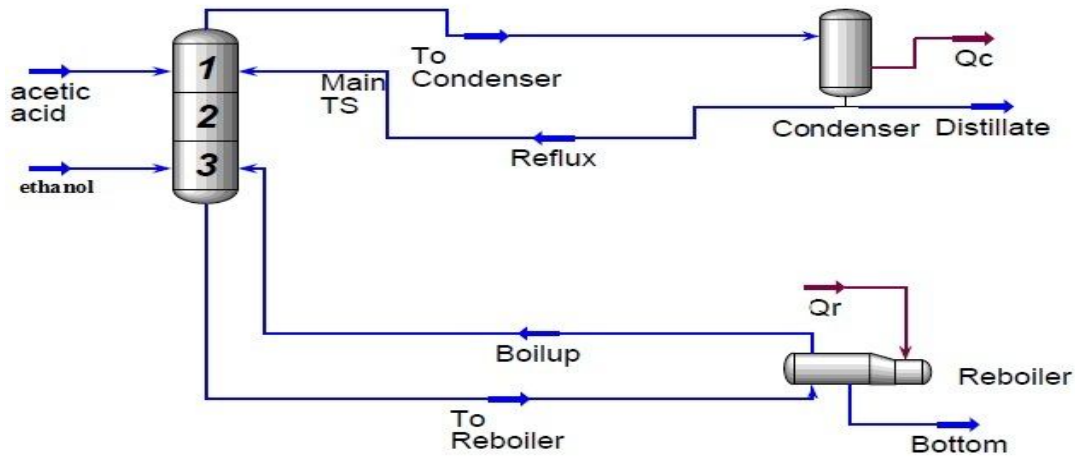


Fig.(1) : Schematic diagram of ethyl acetate reactive distillation column constructed using HYSYS.

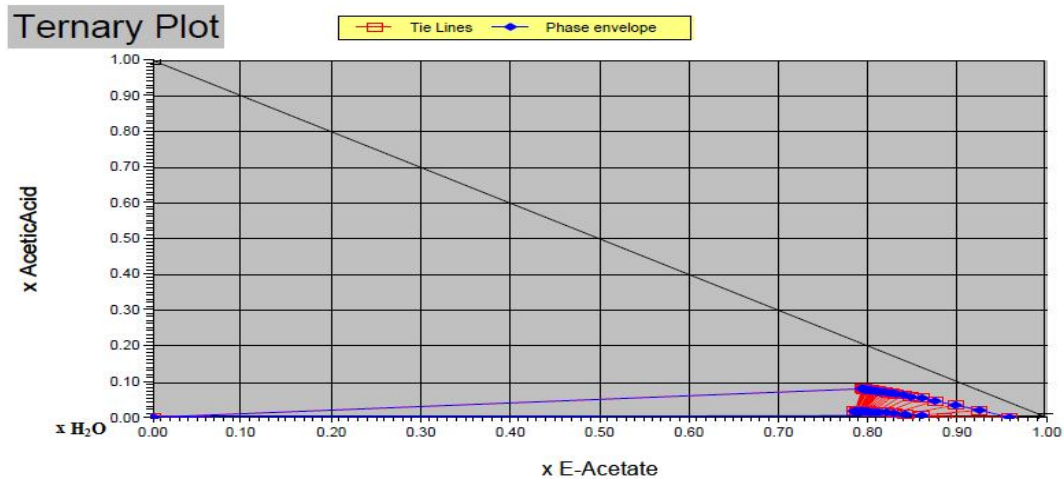


Fig.(2): Residue curve map of (HAc–EtAc–H₂O) system constructed using HYSYS.

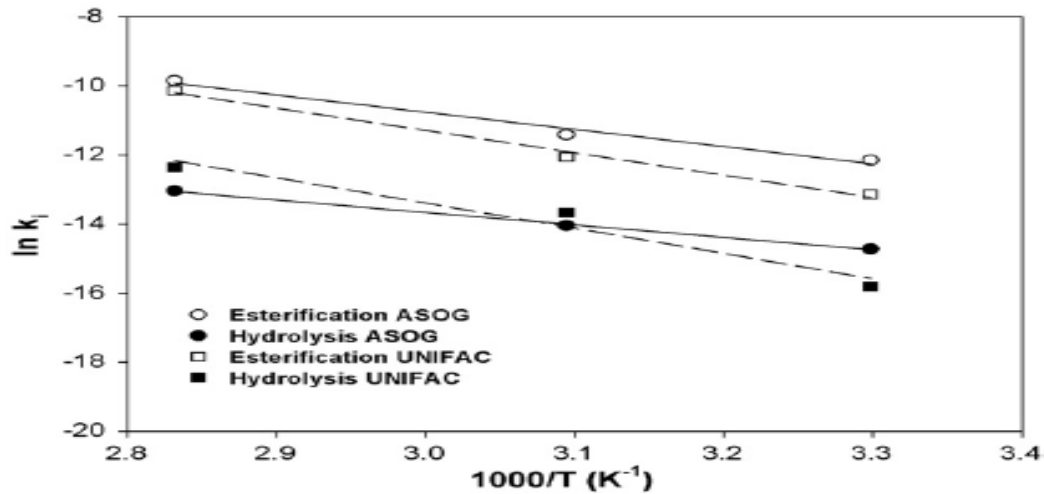


Fig.(3): Arrhenius diagrams of the rate constants for the homogeneous esterification and hydrolysis reactions by Calvar et al. [18].

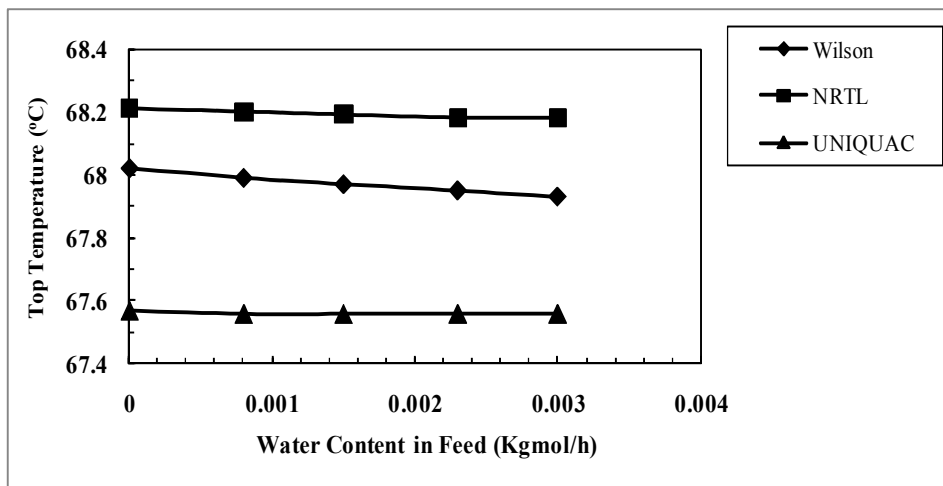


Fig.(4): Effect of Water Content in Feed on Top Temperature at $R=2.5$, $T_b=85^{\circ}C$ with Intermediate Feed.

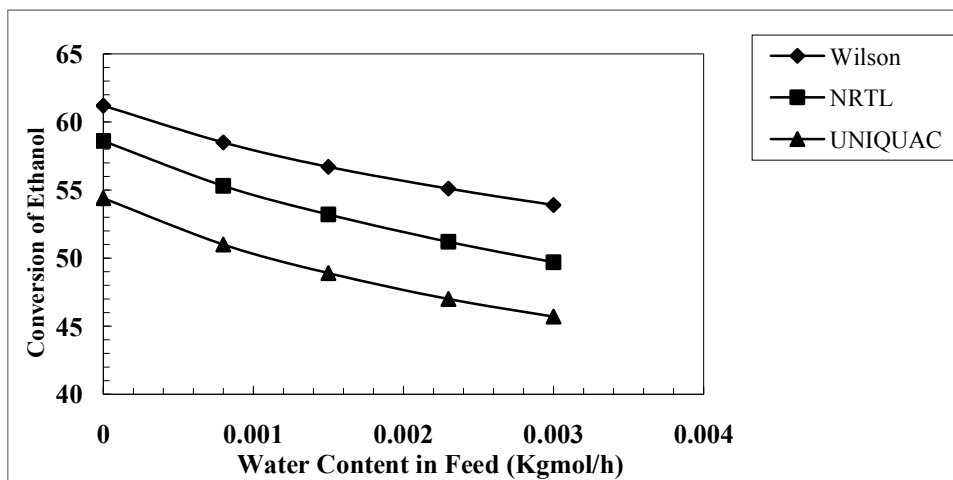


Fig.(5): Effect of Water Content in Feed on Conversion of Ethanol at $R=2.5$, $T_b=85^{\circ}C$ with Intermediate Feed.

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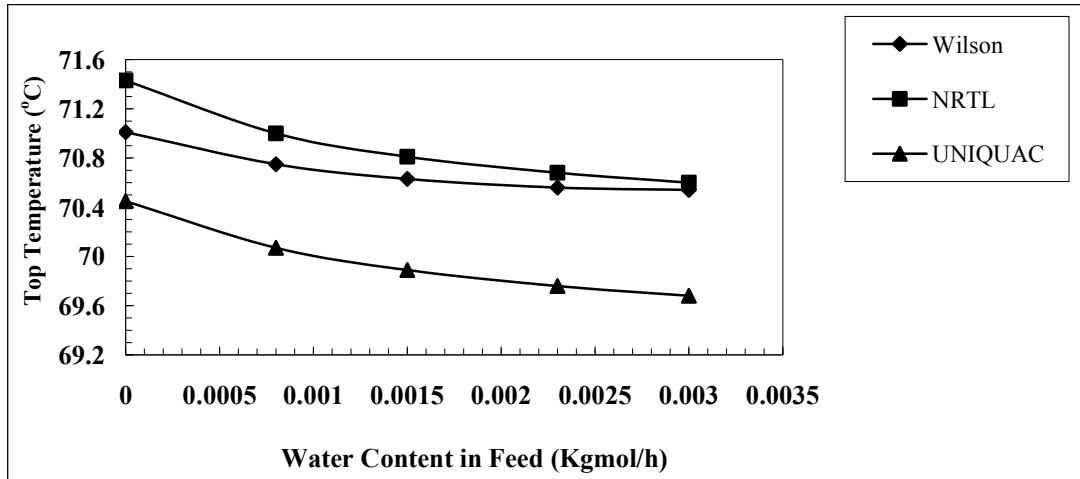


Fig.(6): Effect of Water Content in Feed on Top Temperature at R=2.5, T_b=85°C with Split Feed.

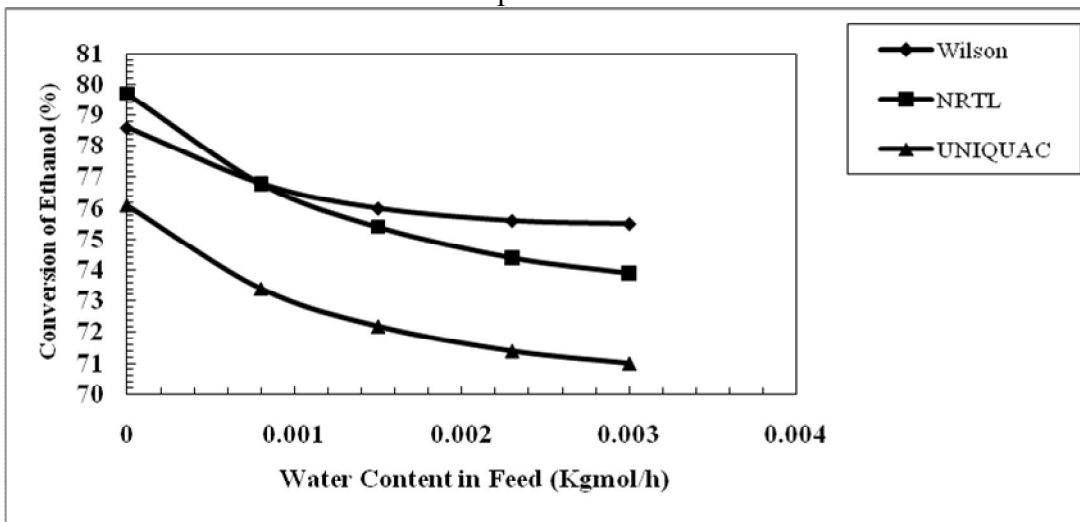


Fig.(7): Effect of Water Content in Feed on Conversion of Ethanol at R=2.5, T_b=85°C with Split Feed.

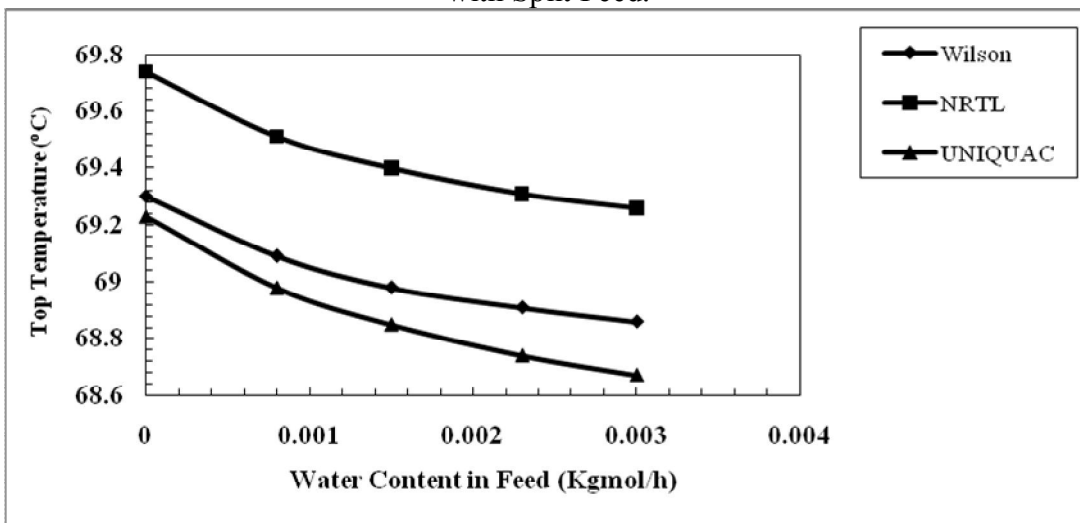


Fig.(8): Effect of Water Content in Feed on Top Temperature at R=2.5, T_b=85°C with Upper Feed.

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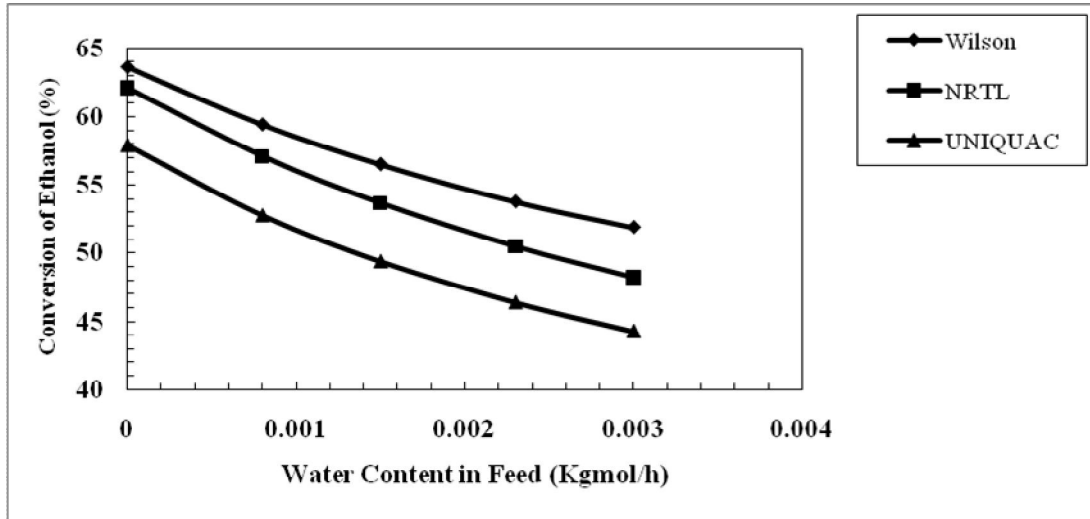


Fig.(9): Effect of Water Content in Feed on Conversion of Ethanol at $R=2.5$, $T_b=85^\circ\text{C}$ with Upper Feed

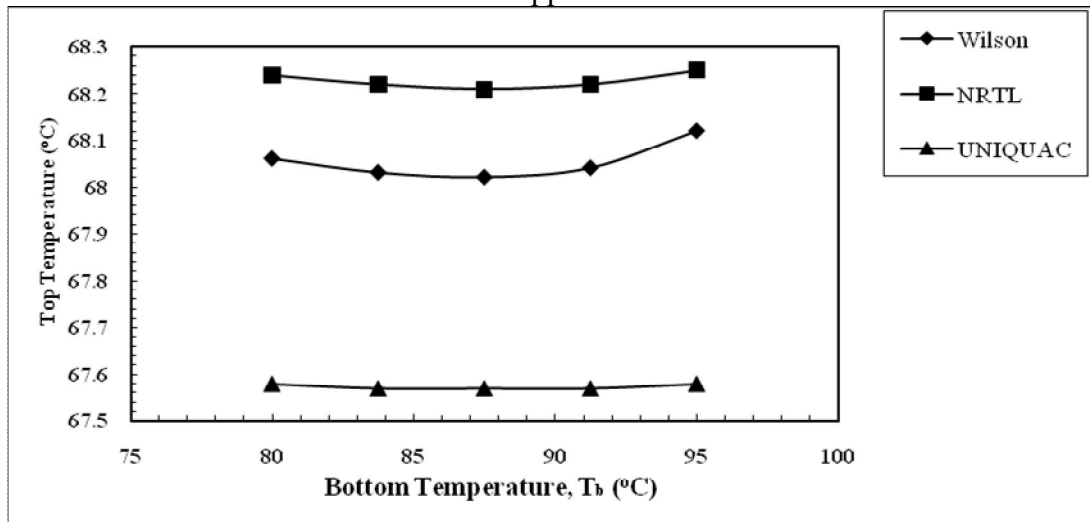


Fig.(10): Effect of Bottom Temperature on Top Temperature at $R=2.5$ without Water Content in Intermediate Feed.

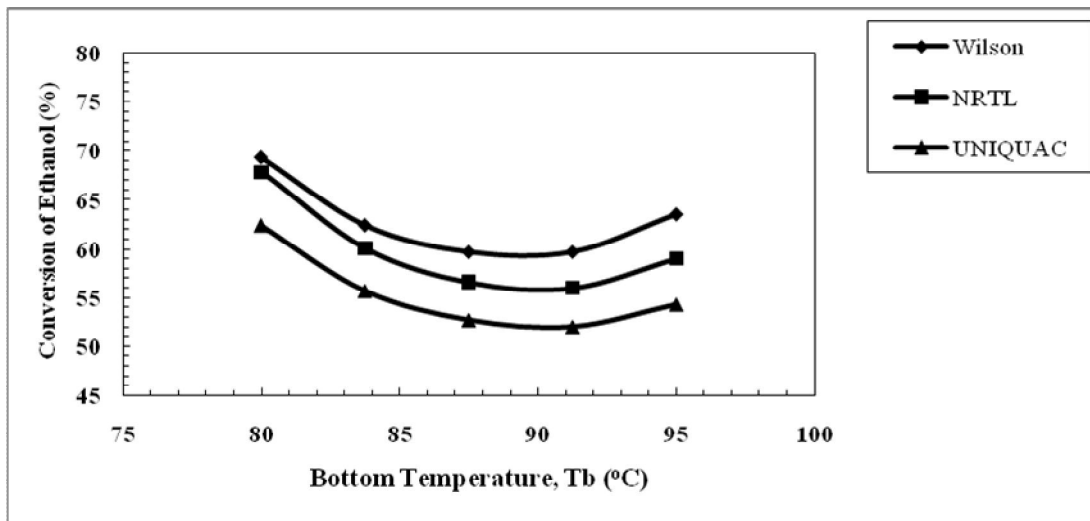


Fig.(11): Effect of Bottom Temperature on Conversion of Ethanol at $R=2.5$ without Water Content in Intermediate Feed.

PROCESS SIMULATION STUDY OF ETHYL ACETATE REACTIVE DISTILLATION COLUMN BY HYSYS® 3.2 SIMULATOR

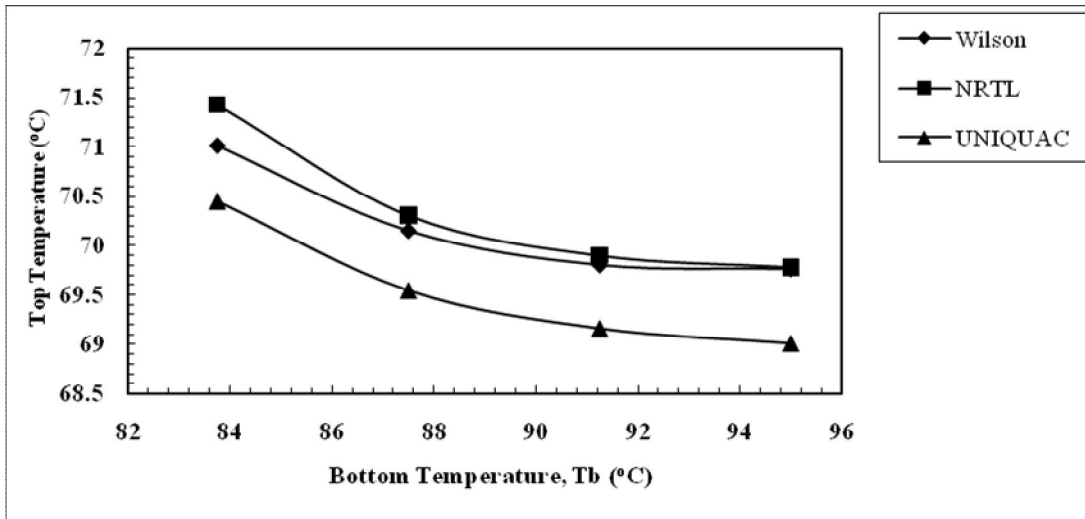


Fig.(12): Effect of Bottom Temperature on Top Temperature at R=2.5 without Water Content in Split Feed.

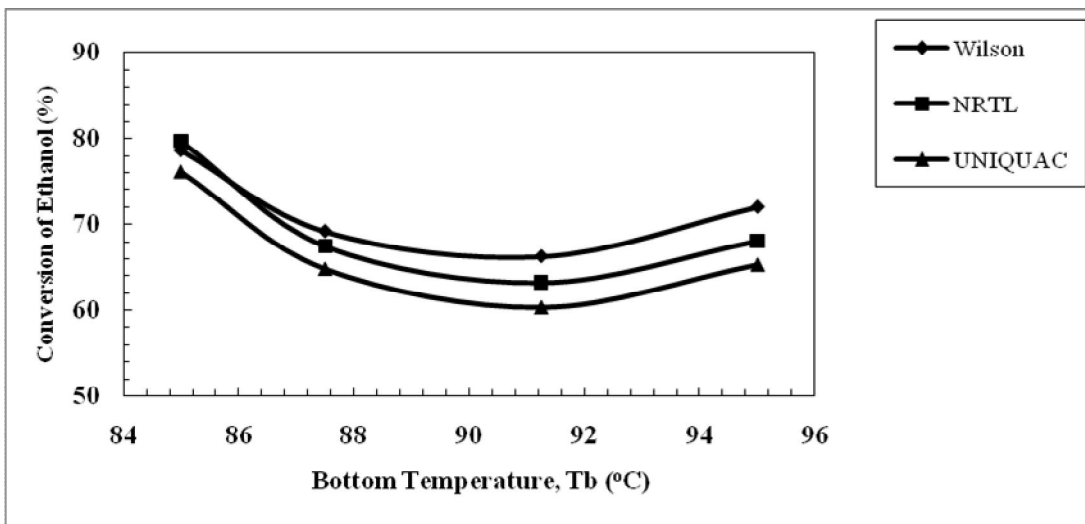


Fig.(13): Effect of Bottom Temperature on Conversion of Ethanol at R=2.5 without Water Content in Split Feed.

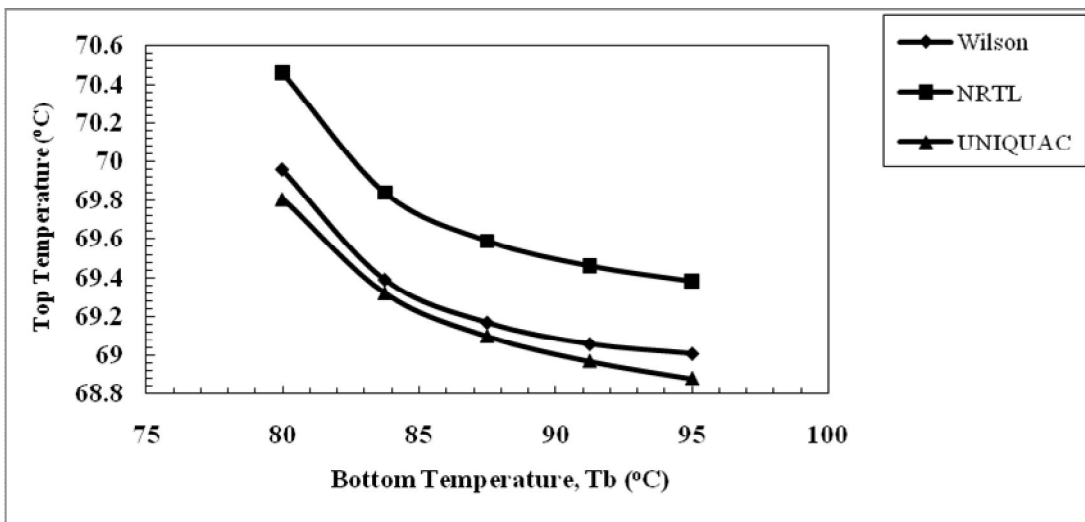


Fig.(14): Effect of Bottom Temperature on Top Temperature at R=2.5 without Water Content in Upper Feed.

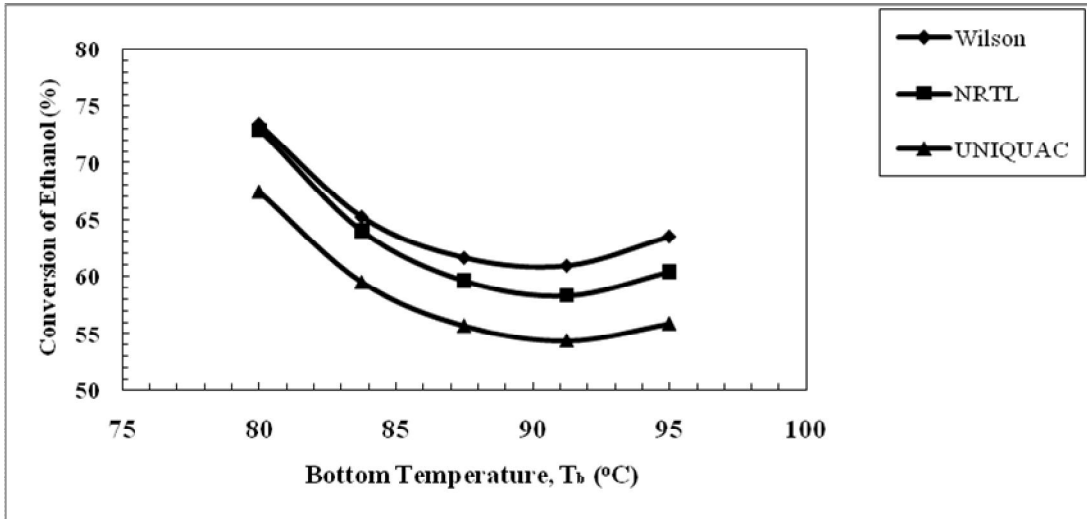


Fig.(15): Effect of Bottom Temperature on Conversion of Ethanol at $R=2.5$ without Water Content in Upper Feed.

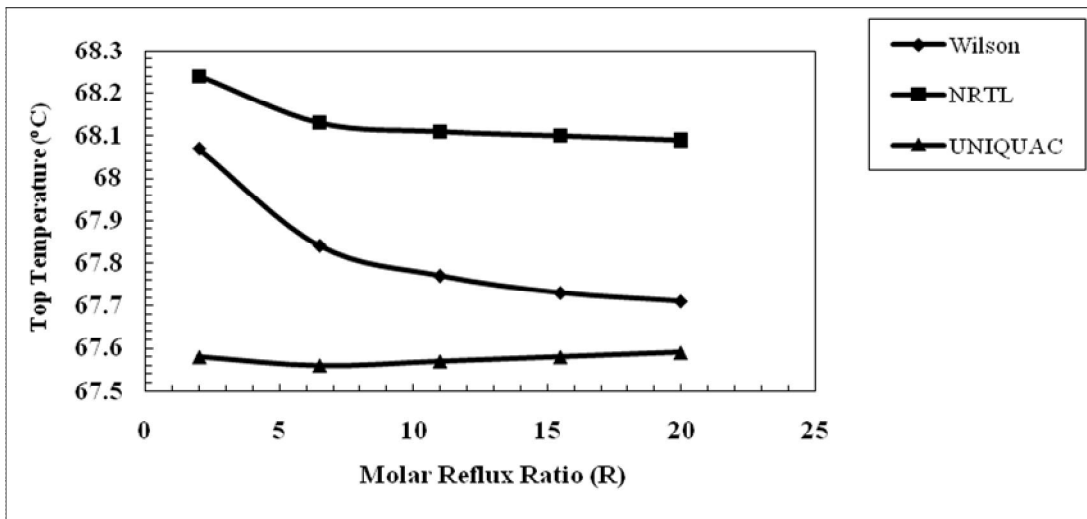


Fig.(16): Effect of Molar Reflux Ratio on Top Temperature at $T_b=85^\circ\text{C}$ without Water Content in Intermediate Feed.

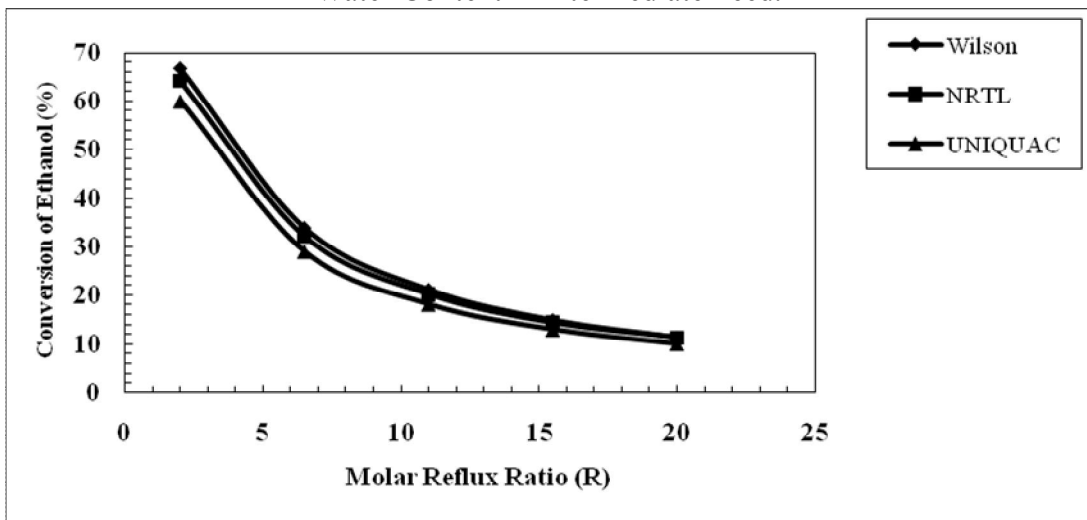


Fig.(17): Effect of Molar Reflux Ratio on Conversion of Ethanol at $T_b=85^\circ\text{C}$ without Water Content in Intermediate Feed.

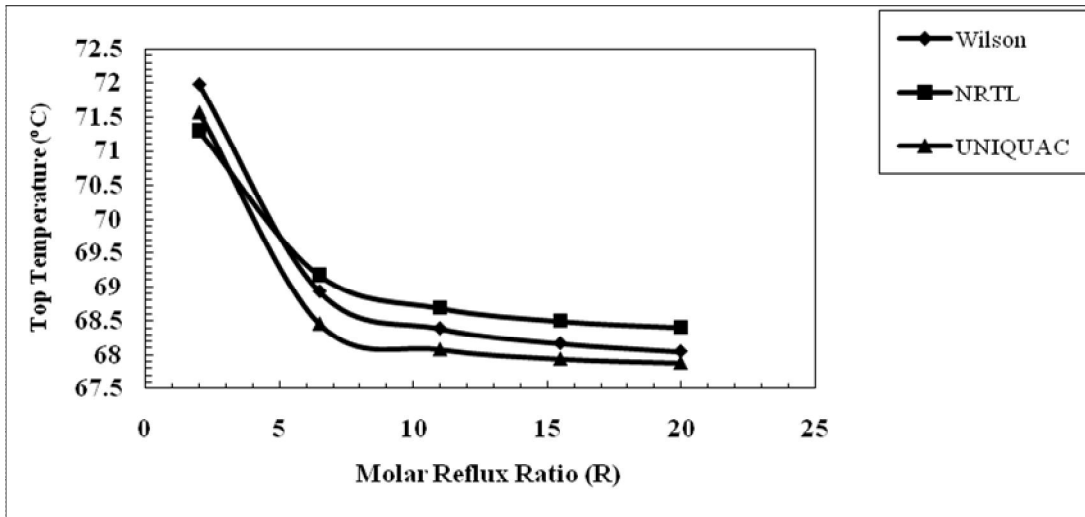


Fig.(18): Effect of Molar Reflux Ratio on Top Temperature at $T_b=85^\circ\text{C}$ without Water Content in Spilt Feed.

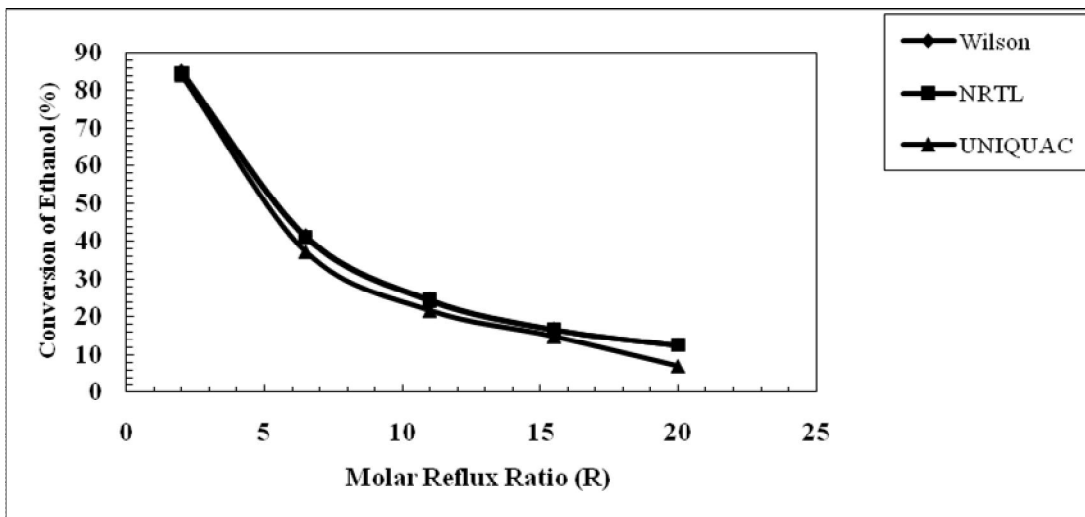


Fig.(19): Effect of Molar Reflux Ratio on Conversion of Ethanol at $T_b=85^\circ\text{C}$ without Water Content in Spilt Feed.

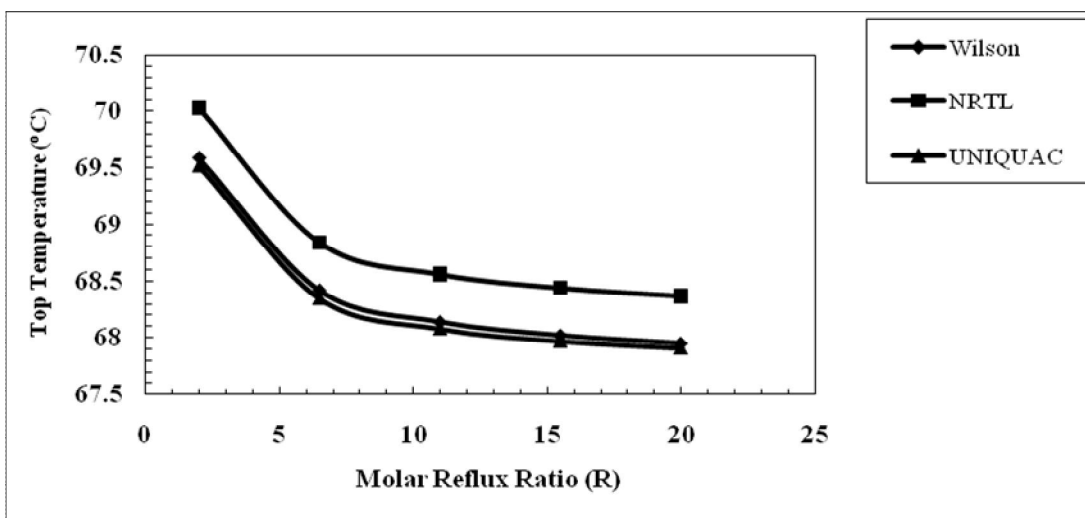


Fig.(20): Effect of Molar Reflux Ratio on Top Temperature at $T_b=85^\circ\text{C}$ without Water Content in Upper Feed.

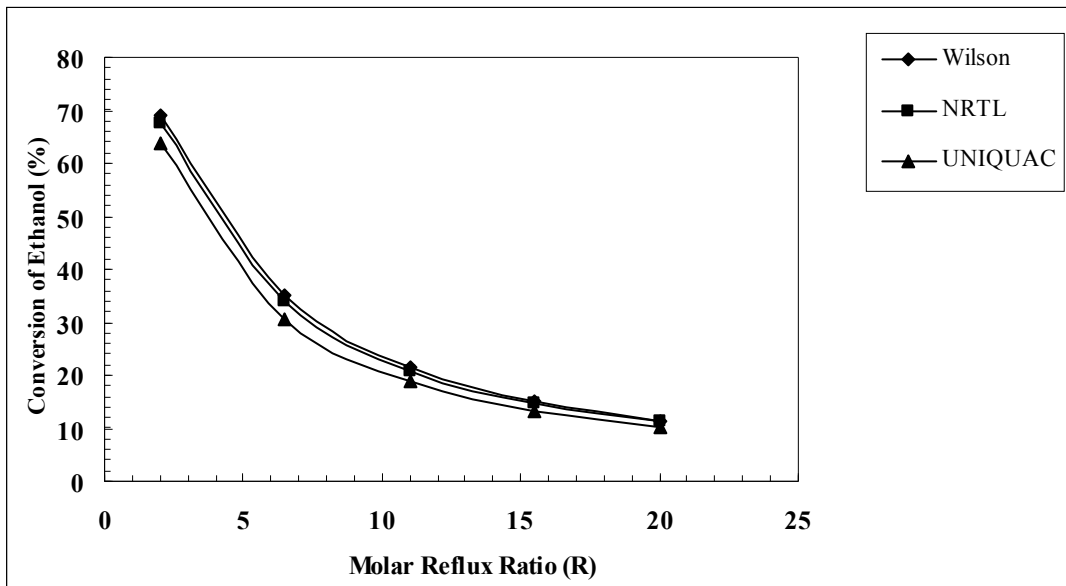


Fig.(21): Effect of Molar Reflux Ratio on Conversion of Ethanol at $T_b=85^{\circ}\text{C}$ without Water Content in Upper Feed.

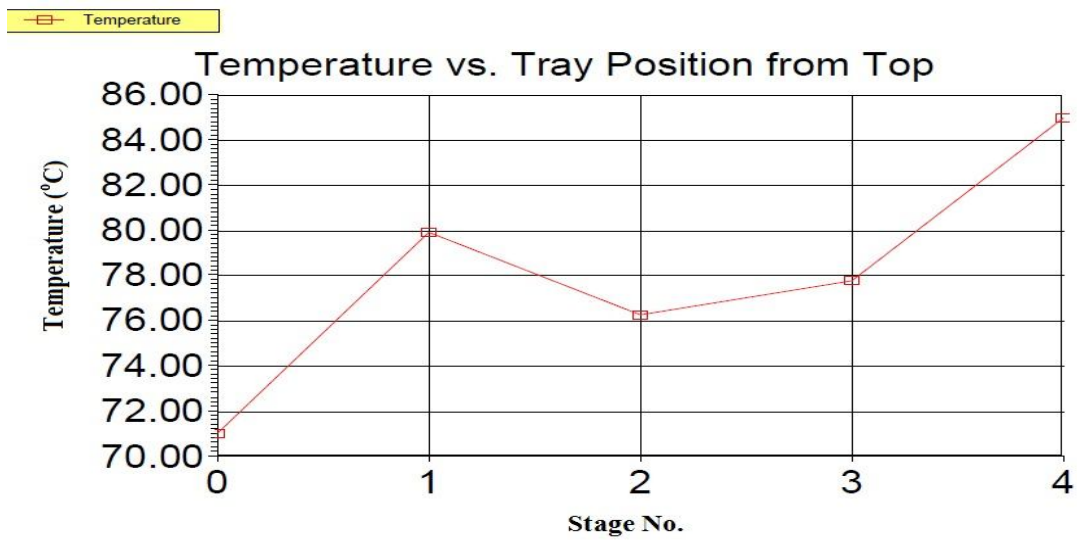


Fig.(22): Temperature Profile of Reactive Distillation Column.

دراسة في المحاكاة النظرية لتحليل عمود التقطير التفاعلي لخلات الأثيل باستخدام برنامج المحاكاة HYSYS® 3.2

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الخلاصة

في هذا البحث تم محاكاة عمود التقطير التفاعلي لإنتاج خلات الأثيل من الأيثانول وحامض الخليك باستخدام برنامج المحاكاة HYSYS. وهذا التقطير التفاعلي عبارة عن عملية واحدة حيث التفاعل والفصل يحدثان بداخل برج تقطير مفرد.

تم حساب الخواص الترموديناميكية باستخدام ثلاث موديلات (NRTL, Wilson, UNIQUA) وهي متوفرة ضمن برنامج HYSYS.

وتم دراسة تأثير كل من درجة حرارة أسفل العمود، المحتوى المائي في المادة الداخلة ونسبة الراجع على درجة حرارة أعلى العمود ونسبة تحول الأيثانول باستخدام هذه الموديلات الثلاث عند حالات المادة الداخلة الثلاث (العلوي، المتوسط، المتجزئ).

وأفضل الظروف التشغيلية التي تم الوصول إليها هي : درجة حرارة أسفل العمود ($83-86^{\circ}\text{C}$)، نسبة الراجع (5-2) بدون محتوى مائي في المادة الداخلة بالحالة المتجزئة باستخدام Wilson كأفضل موديل. هذه الدراسة تعطي دليل على نجاح المحاكاة باستخدام HYSYS بسبب تقارب نتائج المحاكاة مع النتائج العملية للباحث (Calvar)^[19].

الكلمات الدالة:

برنامج المحاكاة HYSYS ، التقطير التفاعلي ، عمليات الأسترة ، إنتاج خلات الأثيل .