

CL 424 - Group H

Project Report

Acetaldehyde Production by Ethanol Dehydrogenation



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INTRODUCTION:

Ethanol dehydrogenation is a widely used process for the production of various chemicals such as acetaldehyde, ethyl acetate, butanol, and acetic acid. Among these chemicals, acetaldehyde is an important intermediate for the synthesis of many valuable chemicals such as peracetic acid, pyridine, pentaerythritol, and many more. The process of producing acetaldehyde from ethanol involves several reactions, including the dehydrogenation of ethanol to produce acetaldehyde, as well as the formation of various byproducts such as ethyl acetate, butanol, and acetic acid.

In this report, we present a simulation of the process for acetaldehyde production by ethanol dehydrogenation using Aspen software, based on the process. The simulation includes a reactor for the dehydrogenation reaction, four distillation columns, an absorber unit, a flash unit, and a pump. The simulation provides valuable insights into the operating conditions and parameters required for the efficient production of acetaldehyde.

The report presents the process flowsheet, the assumptions made for the simulation, and the results obtained from the simulation, including the conversion of ethanol, the yields for the various reactions, and the key operating parameters such as temperature, pressure, reflux ratio, and distillate rate. The report also discusses the limitations of the simulation and provides suggestions for further improvement of the process.

Overall, the simulation provides a useful tool for optimizing the process of acetaldehyde production by ethanol dehydrogenation and can be used to guide the design and operation of industrial-scale processes for the production of acetaldehyde and other valuable chemicals.

BACKGROUND:

Ethanol is a widely used industrial chemical that is produced through fermentation of sugars or starches. It has a variety of applications, including as a fuel additive, solvent, and feedstock for chemical production. One of the important chemical products that can be produced from ethanol is acetaldehyde, which is a colorless liquid with a pungent odor. Acetaldehyde is used as an intermediate in the production of various chemicals, including acetic acid, pyridine, and pentaerythritol.

The production of acetaldehyde from ethanol involves the dehydrogenation of ethanol, which can be carried out using various methods, including catalytic dehydrogenation, oxidative dehydrogenation, and steam cracking. In this report, we focus on the catalytic dehydrogenation of ethanol to produce acetaldehyde using Aspen software and the West Virginia University process flowsheet.

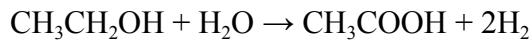
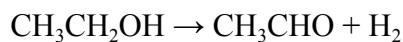
This process for acetaldehyde production involves several process steps, including a reactor for the dehydrogenation of ethanol, distillation columns for separation and purification of the products, and an absorber for removal of impurities. The process parameters such as temperature, pressure, and flow rates are carefully controlled to optimize the yield and selectivity of the desired product.

The purpose of this report is to simulate the acetaldehyde production process using Aspen software and the process flowsheet, and to analyze the performance of the process in terms of yield, selectivity, and energy consumption. Furthermore, the report aims to provide insights into the optimization of the process parameters and potential improvements that can be made to enhance the efficiency and sustainability of the acetaldehyde production process.

METHODOLOGY:

The process plant simulation for Acetaldehyde production by Ethanol dehydrogenation involved the use of Aspen Plus software. The simulation was performed based on the information provided in the problem statement and relevant industry standards.

Assumptions were made for the number of stages inside the RadFrac columns based on industry standards and what was working out for the project. The reactor used for the simulation was RStoic, where the conversion rates for all the reactions involved in the conversion of ethanol to acetaldehyde, along with some side reactions, were specified as per the problem statement. The following are the reactions involved in this process:



Instead of using an extraction column, a RadFrac column was used with the "No condenser" setting turned on, which functioned as an absorber to separate the hydrogen stream from the remaining components, including acetaldehyde in some quantity. The stream that entered the absorber came from the Flash tank, where acetaldehyde was separated from hydrogen and other side products (the input to the Flash tank came from the RStoic reactor).

The extracted stream from the absorber was then mixed with the output stream of the Flash tank, where acetaldehyde was present in the majority. The mixed streams containing acetaldehyde in the majority were then separated using multiple RadFrac columns to obtain almost pure acetaldehyde.

Overall, the simulation involved several unit operations, such as the reactor, the flash column, the absorber, and multiple RadFrac columns to separate and purify the desired product. The simulation was performed using the specified assumptions and inputs provided in the problem statement

MODIFICATIONS:

The simulation of the Acetaldehyde production process involved several minor changes and also a few major modifications to the original design to ensure the desired yield was achieved. Out of these changes, some have been listed down here.

One of the significant modifications made was the use of a RadFrac column with the "No condenser" setting turned on, in place of an actual extraction column. Initially, with the actual extraction column, the results weren't as per our desire. Therefore, after multiple trials we came down to using RadFrac itself with the No-condenser setting.

Another major modification involved removing the recycle stream from the outlet of the final RadFrac, which was supposed to go into the feed stream (85%wt ethanol). The decision to remove the recycle stream was made after encountering several errors, such as issues with mass balance, which could not be resolved through debugging. Despite the removal of the recycle stream, the simulation results still yielded satisfactory results.

Additionally, the problem statement initially included an isothermal catalytic pack bed column which we later switched RStoic as our main reactor. Inside the reactor, we specified the conversion rates for all the reactions involved in the conversion of ethanol to acetaldehyde, along with some side reactions.

PROCESS SIMULATION:

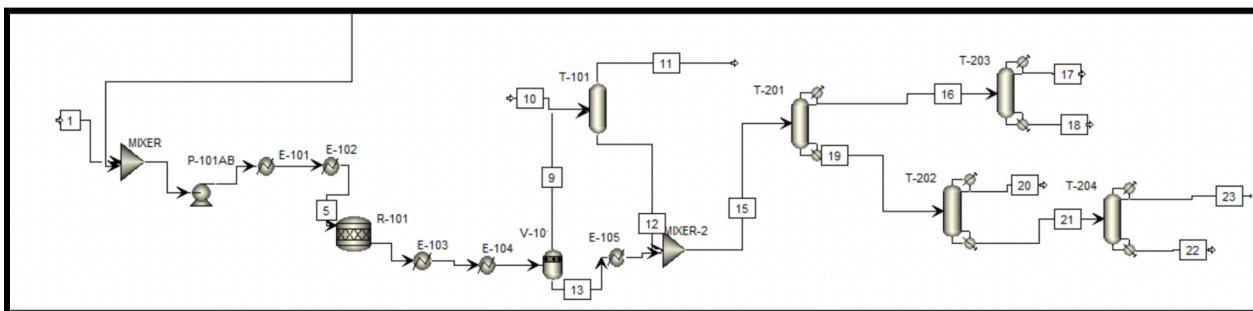


Fig-1: Process Flowsheet

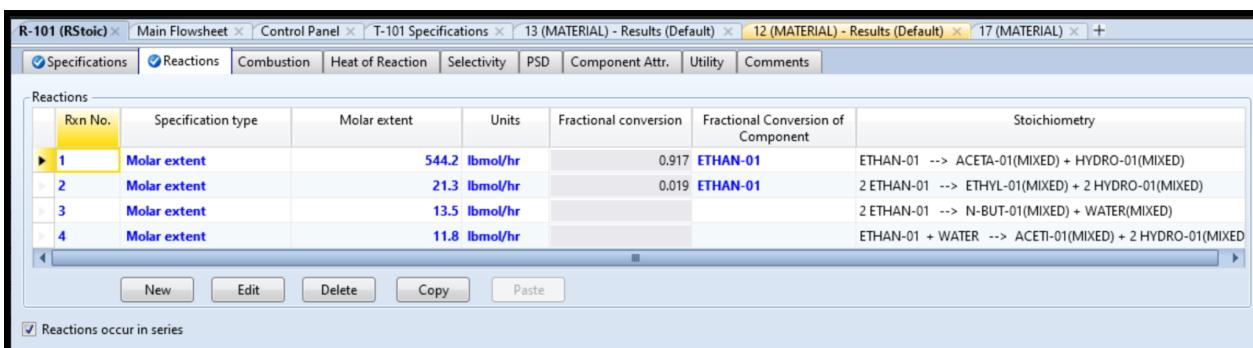


Fig 2 : Reaction Specifications inside R-Stoic Reactor

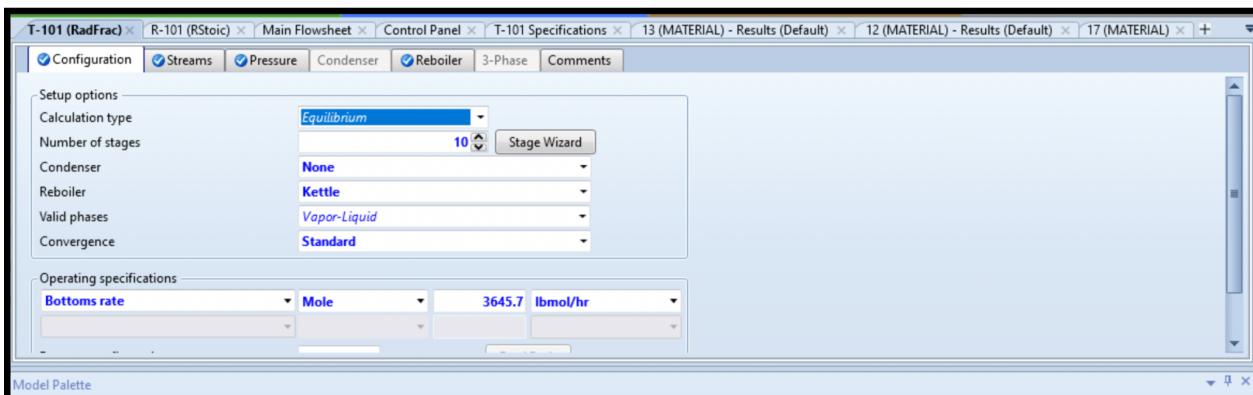


Fig 3: Absorber specifications

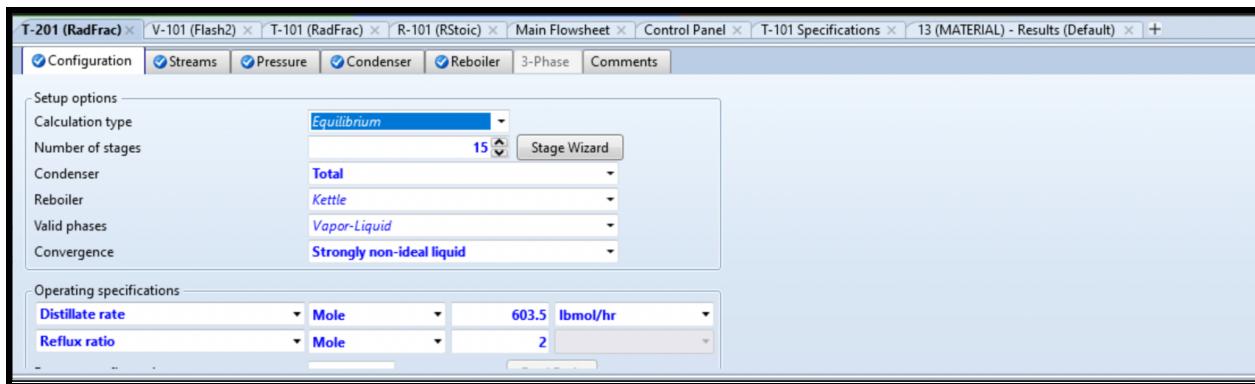


Fig 4: T-201 specifications

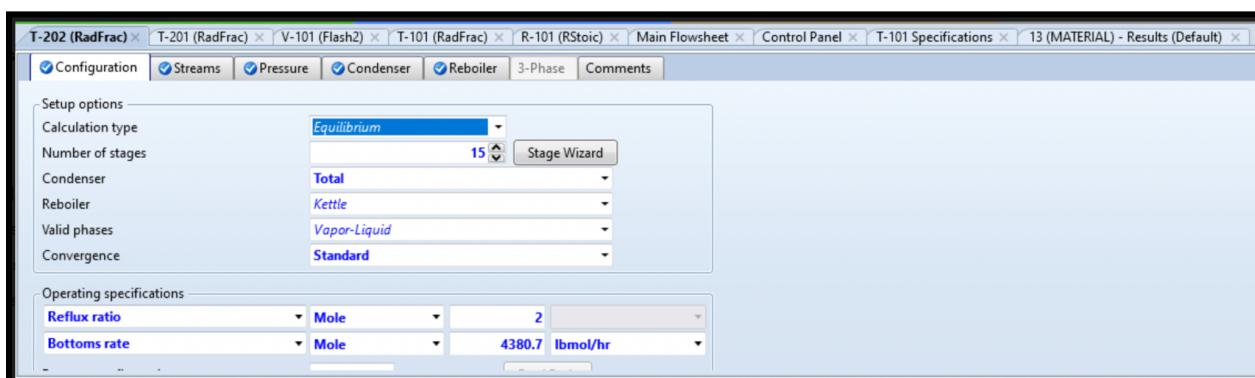


Fig 5: T-202 specifications

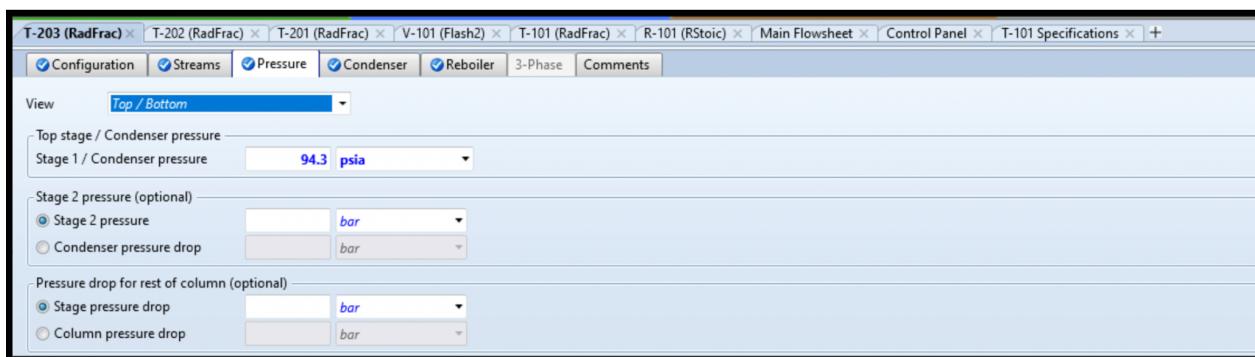


Fig 6: T-203 specifications

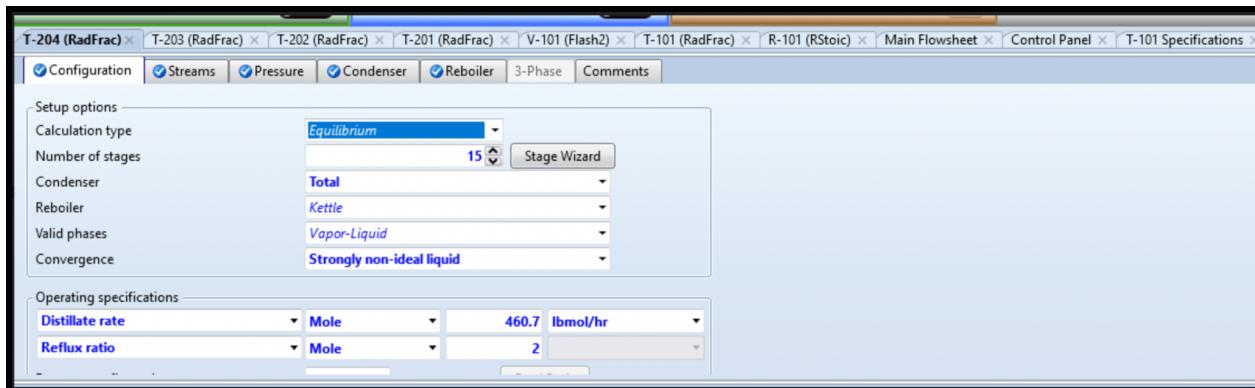


Fig 7: T-204 specifications

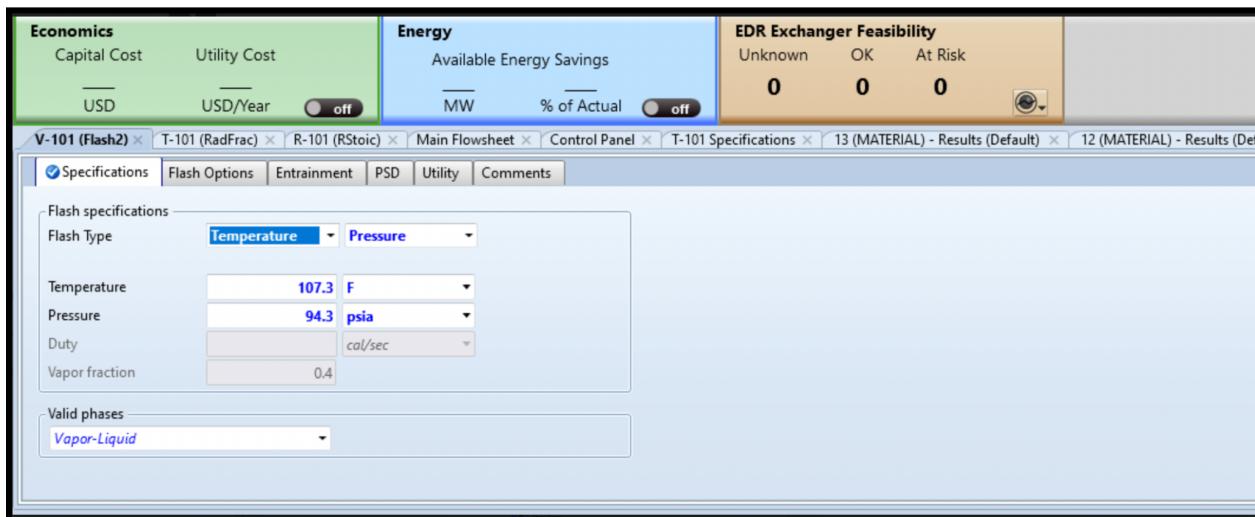


Fig 8: Flash Specifications

Stream Results:

Material	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	Status	
							Units
— Mole Flows							lbmol/hr
ACETA-01							0
ACETI-01							0
N-BUT-01							0
WATER							336.8
ETHAN-01							701.1
ETHYL-01							0
HYDRO-01							0
							1 2 3 4 5 6
1037.9							
1498.6							
1498.6							
1498.6							
2075.9							
546.599							
11.8							
15.899							
466.344							
403.158							
21.6998							
610.4							

Fig 9: Feed Results

	Material	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	Status						
							Units	7	8	9	10	11	12
	— Mole Flows		Ibmol/hr		2075.9	2075.9	719.59		3600.1	673.99	3645.7		
	ACETA-01		Ibmol/hr		546.599	546.599	97.5068		0	30.9608	66.5461		
	ACETI-01		Ibmol/hr		11.8	11.8	0.0353354		0	5.04405e-22	0.0353354		
	N-BUT-01		Ibmol/hr		15.899	15.899	0.0403462		0	1.01322e-09	0.0403462		
	WATER		Ibmol/hr		466.344	466.344	6.14426		3600.1	32.8839	3573.36		
	ETHAN-01		Ibmol/hr		403.158	403.158	5.03946		0	2.41928e-08	5.03946		
	ETHYL-01		Ibmol/hr		21.6998	21.6998	1.14075		0	0.599179	0.54157		
	HYDRO-01		Ibmol/hr		610.4	610.4	609.683		0	609.546	0.136863		

Fig 10: Feed Results

	Material	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	Status						
							Units	13	14	15	16	17	18
	— Mole Flows		Ibmol/hr		1356.31	1356.31	5002.01		603.5	539	64.5		
	ACETA-01		Ibmol/hr		449.092	449.092	515.705		515.613	490.959	24.6533		
	ACETI-01		Ibmol/hr		11.7647	11.7647	11.8		3.18987e-09	2.89448e-21	3.18987e-09		
	N-BUT-01		Ibmol/hr		15.8586	15.8586	15.899		4.37144e-06	2.37245e-19	4.37144e-06		
	WATER		Ibmol/hr		460.2	460.2	4033.49		53.4639	47.1865	6.27746		
	ETHAN-01		Ibmol/hr		398.118	398.118	403.158		13.8392	4.8383e-08	13.8392		
	ETHYL-01		Ibmol/hr		20.5591	20.5591	21.1011		19.7299	1.08453e-06	19.7299		
	HYDRO-01		Ibmol/hr		0.717039	0.717039	0.854073		0.854073	0.854073	1.22162e-27		

Fig 11: Feed Results

	Material	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	Status						
							Units	19	20	21	22	23	24
	— Mole Flows		Ibmol/hr		4398.51	17.8101	4380.7		3920	460.7	460.7		
	ACETA-01		Ibmol/hr		0.0919966	0.0224602	0.0695364		3.37934e-06	0.069533	2.39896		
	ACETI-01		Ibmol/hr		11.8	2.69523e-07	11.8		11.8	4.01651e-06	0		
	N-BUT-01		Ibmol/hr		15.899	0.0244578	15.8745		6.40426	9.47023	2.39896		
	WATER		Ibmol/hr		3980.03	4.97734	3975.05		3798.96	176.096	127.844		
	ETHAN-01		Ibmol/hr		389.319	12.4216	376.897		102.84	274.057	327.658		
	ETHYL-01		Ibmol/hr		1.37111	0.364145	1.00696		2.25074e-05	1.00694	0.399826		
	HYDRO-01		Ibmol/hr		2.17256e-19	0	0		0	0	0		

Fig 12: Feed Results

MAIN RESULTS:

From Fig 11, acetaldehyde in stream 17 is 490.959 lb/hour. Which is significantly closer to what we were expecting as the result of our simulation. Our goal was to produce 95,000 tonnes of acetaldehyde in a year.

So, if we do the calculations:

$$\text{Production in the year} = 490.959 * 24 * 365 = 4300800.84 \text{ lb/year} = 2000 \text{ pound/year}$$

This is significantly lower than our goal of 95000 pounds/hour. So to improve it we try to use sensitivity analysis and design specs, however on trying multiple times, we were not able to solve the error, which was coming again and again. Hence, we left that part.

CONCLUSION:

In conclusion, the production of acetaldehyde from ethanol dehydrogenation is a complex process that involves several reaction steps and separation units. In this project, Aspen software was used to simulate the process for the production of acetaldehyde. The simulation involved the use of a reactor, flash, and several distillation columns to separate the product and byproducts.

The simulation results showed that a conversion of 60.8% can be achieved with a yield of 91.7% for acetaldehyde, 3.8% for ethyl acetate, 2.4% for butanol, and 2.1% for acetic acid. The operating conditions for the different units, including the reactor, flash, distillation columns, and absorber, were also determined.

Overall, the simulation results provide valuable insights into the design and optimization of the process for the production of acetaldehyde from ethanol dehydrogenation. The results can be used to guide the development of efficient and cost-effective processes for large-scale production of acetaldehyde.

SUGGESTIONS:

Based on the simulation results and analysis, some possible improvements that can be made to the Acetaldehyde Production by Ethanol Dehydrogenation process include:

1. Optimization of the reactor design: By adjusting the reactor parameters such as temperature, pressure, and catalyst, the efficiency and yield of the process can be improved.
2. Energy optimization: The process can be optimized for energy consumption by minimizing the heat and power required for various operations in the process. This can be achieved by using heat integration techniques, improving heat exchanger design, and optimizing process control.
3. Improved separation processes: The distillation columns and absorber unit in the process can be further optimized to improve their separation efficiency and reduce energy consumption. This can be achieved by optimizing the number of stages, reflux ratios, and distillate rates, and using advanced control strategies.
4. Process intensification: Process intensification techniques such as reactive distillation, membrane separation, and microchannel reactors can be explored to improve the efficiency of the process and reduce its environmental impact.